

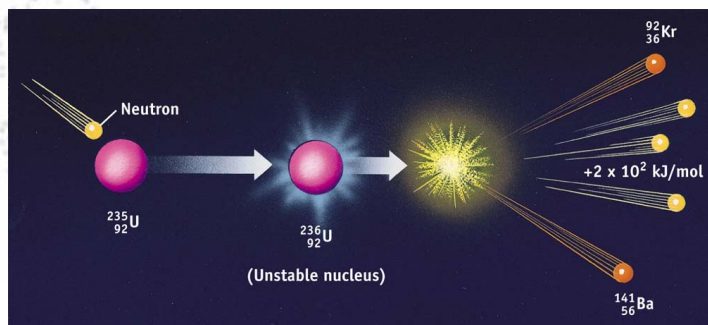
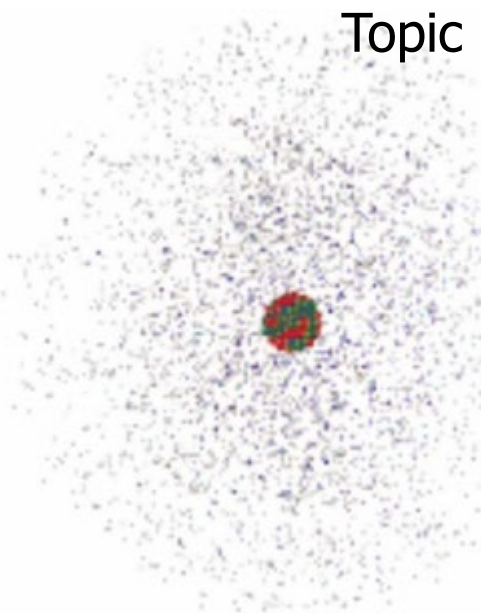
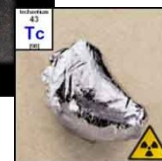
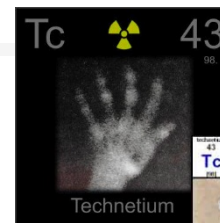


CHEMISTRY 1000

Topic #1: Atomic Structure and Nuclear Chemistry Fall 2020

Dr. Susan Findlay

See Exercises 4.1 to 4.3



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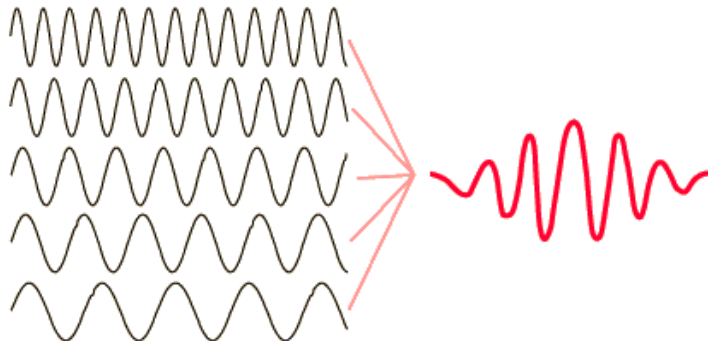
Heisenberg's Uncertainty Principle

- Electrons have wave-particle duality, but it is impossible to show an electron behaving as a wave and a particle at the same time.
- In the 1920s, Werner Heisenberg showed that it's also impossible to know the precise location and momentum of an electron at the same time (because of wave-particle duality):

- A matter wave's momentum can be determined very accurately if we're not concerned about the exact location of the corresponding particle:



- If we're willing to sacrifice some information about the momentum of the wave (by treating the electron as a packet of waves), we can gain more information about the location of the electron:





Heisenberg's Uncertainty Principle

- Thus, if we're willing to accept more uncertainty about an electron's momentum, we can have more certainty in knowing its position – and vice versa. This inverse relationship can be described mathematically:

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

where Δx is the uncertainty about position, Δp is the uncertainty about momentum (i.e. difference between maximum and minimum possible momentum values), and h is Planck's constant.

- Scientists often use \hbar to stand for $h/2\pi$, so this formula can also be written as:

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Heisenberg is scheduled to give a lecture at MIT, but he's running late and speeding through Cambridge in his rental car. A cop pulls him over, and says, "Do you have any idea how fast you were going?" "No," Heisenberg replies brightly, "but I know where I am!"¹

¹ an old joke quoted from Natalie Angier's **The Canon: A Whirligig Tour of the Beautiful Basics of Science** (2007)



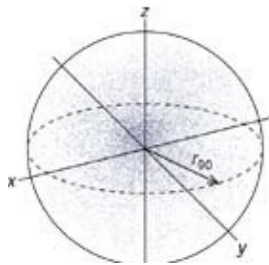
Heisenberg's Uncertainty Principle

- Note that Heisenberg's uncertainty principle is only relevant when discussing extremely small particles such as electrons. Why?

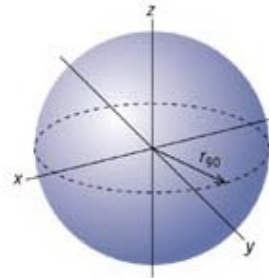
- What does Heisenberg's uncertainty principle mean to the structure of an atom?

So, Where is the Electron?

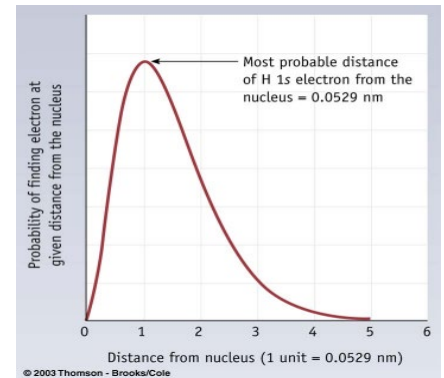
- We may not know the exact location of an electron, but we do know where it's most likely to be found. In fact, an orbital describes exactly that. **An orbital is a wavefunction describing the probability of finding an electron in a given region of space** (*according to the Schrödinger equation*).
- There are different ways to show an orbital:



An electron 'dot' picture is like a time-lapse photo of an electron's position if it is considered to act as a particle for each 'snapshot'



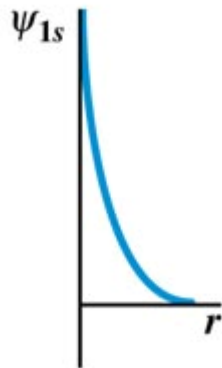
A probability surface shows a 'skin' that encompasses some percentage (often 90% or 95%) of the electron density



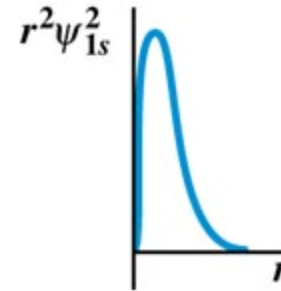
A "radial probability density plot" shows the likelihood of finding an electron at any given distance from the nucleus.

So, Where is the Electron?

- The density of electrons in the electron 'dot' picture increases as the distance to the nucleus decreases (see wavefunction at left), so why is the shape of the electron density plot different?



VS





How do we Describe an Orbital?

- Every orbital in an atom is uniquely described by three quantum numbers:
 - The **principal quantum number** (n) describes the orbital's **energy** (and therefore its size) and the **shell** it occupies.

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

- The **angular momentum quantum number** (l) describes the orbital's **shape** and the **subshell** it occupies.

$$L^2 = l(l + 1)\hbar^2$$

- The **magnetic quantum number** (m_l) identifies the specific orbital within a subshell.

$$L_z = m_l \hbar$$

How do we Describe an Orbital?

- The allowed values for l depend on n and the allowed values for m_l depend on l :

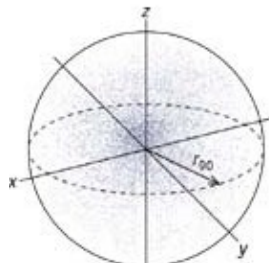
n	l	m_l	<i>total number of orbitals</i>
1	0	0	1
2	0	0	1 + 3 = 4
	1	-1, 0, +1	
3	0	0	1 + 3 + 5 = 9
	1	-1, 0, +1	
	2	-2, -1, 0, +1, +2	
4	0	0	1 + 3 + 5 + 7 = 16
	1	-1, 0, +1	
	2	-2, -1, 0, +1, +2	
	3	-3, -2, -1, 0, +1, +2, +3	

How many different orbitals exist for $n = 5$? $n = 6$? $n = 7$?

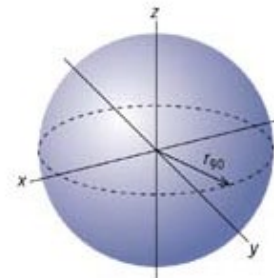
How many different orbitals exist for ($n = 6, l = 4$)?

What do Orbitals Look Like?

- A hydrogen atom is spherical, and all of the orbitals predicted by the Schrödinger equation fit into this sphere.
- Just as 2-dimensional waves have nodes, so can 3-dimensional waves. Each atomic orbital has _____ nodes. _____ of these nodes are **planar**; the rest are **radial**.
- ***s* orbitals ($l = 0$)**
 - An *s* orbital has ___ planar nodes.
 - The simplest orbital has quantum numbers $n = 1, l = 0, m_l = 0$ {abbreviated as $(1,0,0)$ }. This orbital is called $\Psi_{1,0,0}$ or *1s*.
 - We have already seen pictures of a *1s* orbital:



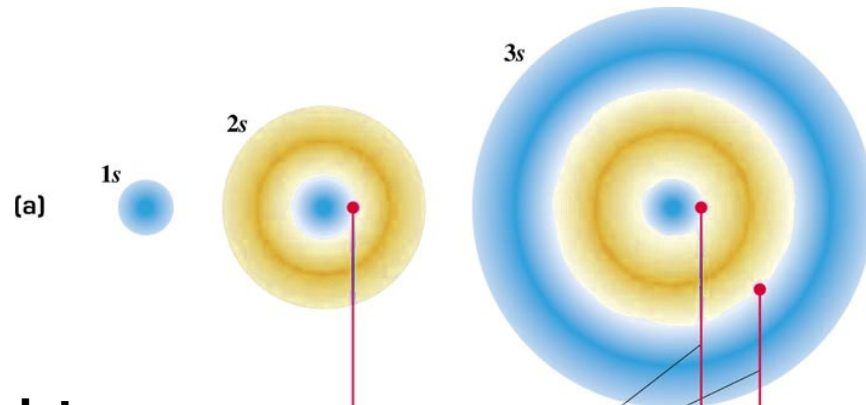
or



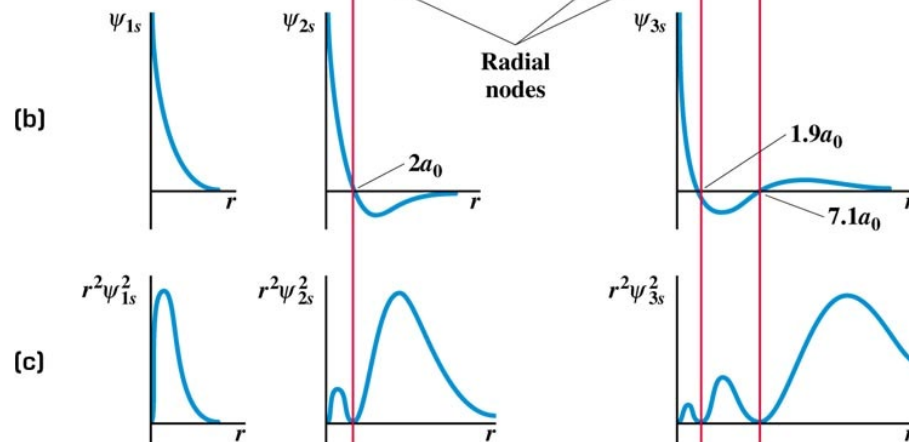
What do Orbitals Look Like?

- The $1s$ orbital has no nodes; however, the higher energy s orbitals have radial nodes, as shown below:

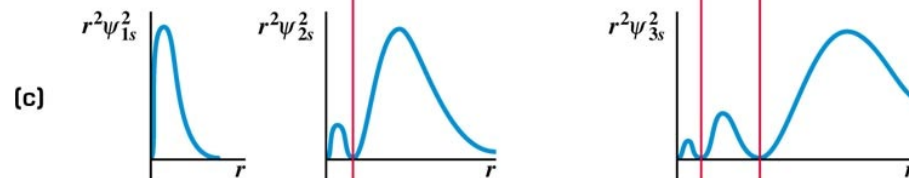
'Dot' diagrams



Wave amplitude plots

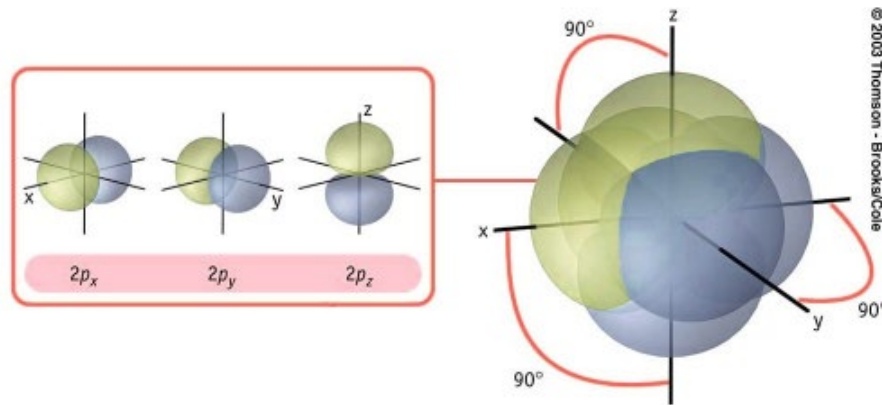


Radial probability density plots



What do Orbitals Look Like?

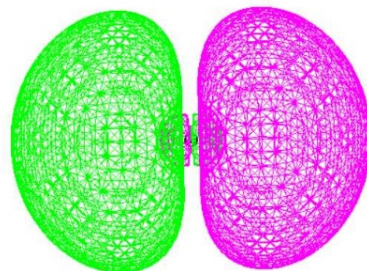
- **p orbitals ($l = 1$)**
 - A p orbital has ___ planar node.



- The orientation of the x, y and z axes is arbitrary unless it is imposed by a magnetic field (hence “magnetic quantum number” for m_ℓ), and there is no direct correlation between m_ℓ and direction. We arbitrarily assign the ‘positive’ phase to be the positive direction on an axis and the ‘negative’ phase to be a negative direction.
- The three p orbitals in a shell pack together to make a perfect sphere. This is because they are _____ functions.

What do Orbitals Look Like?

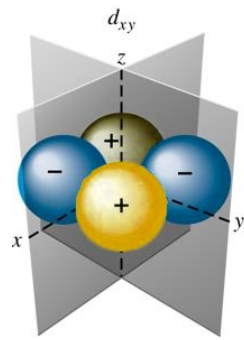
- The higher p orbitals ($3p$, $4p$, etc.) have radial nodes in addition to the nodal plane through the nucleus. Imagine one or more dumbbells tucked concentrically inside the outer dumbbell:



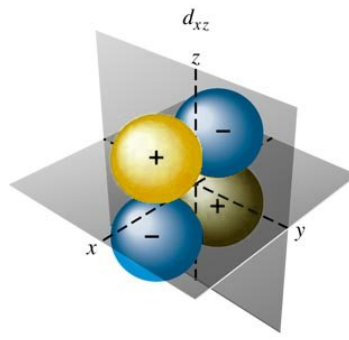
- **d orbitals ($l = 2$)**

- A d orbital has ____ planar nodes.
- For four of the d orbitals, both of these nodes are planes, giving a 'petal-shaped' orbital. For the fifth d orbital (____), the nodes look more like a pair of inverted cones. This gives an orbital that looks a bit like a p orbital with a doughnut around it. (Note the phases, though; they are different from a p orbital.)
- The higher energy d orbitals ($4d$, $5d$, etc.) also have radial nodes.

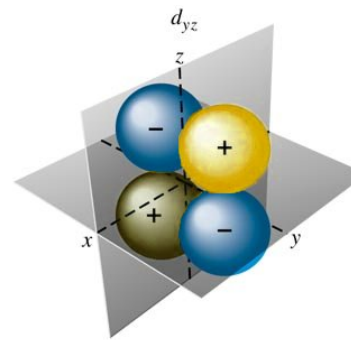
What do Orbitals Look Like?



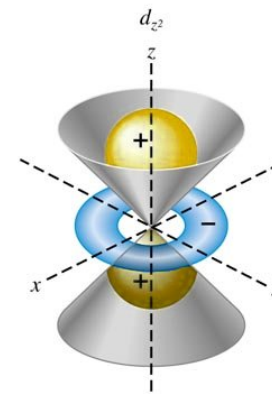
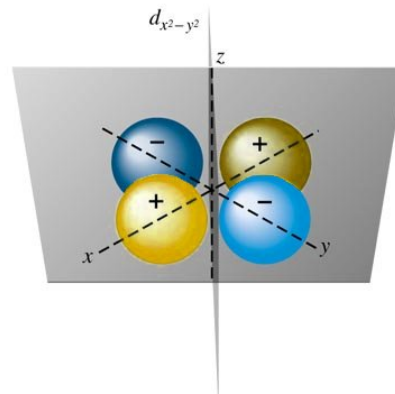
(a)



(b)

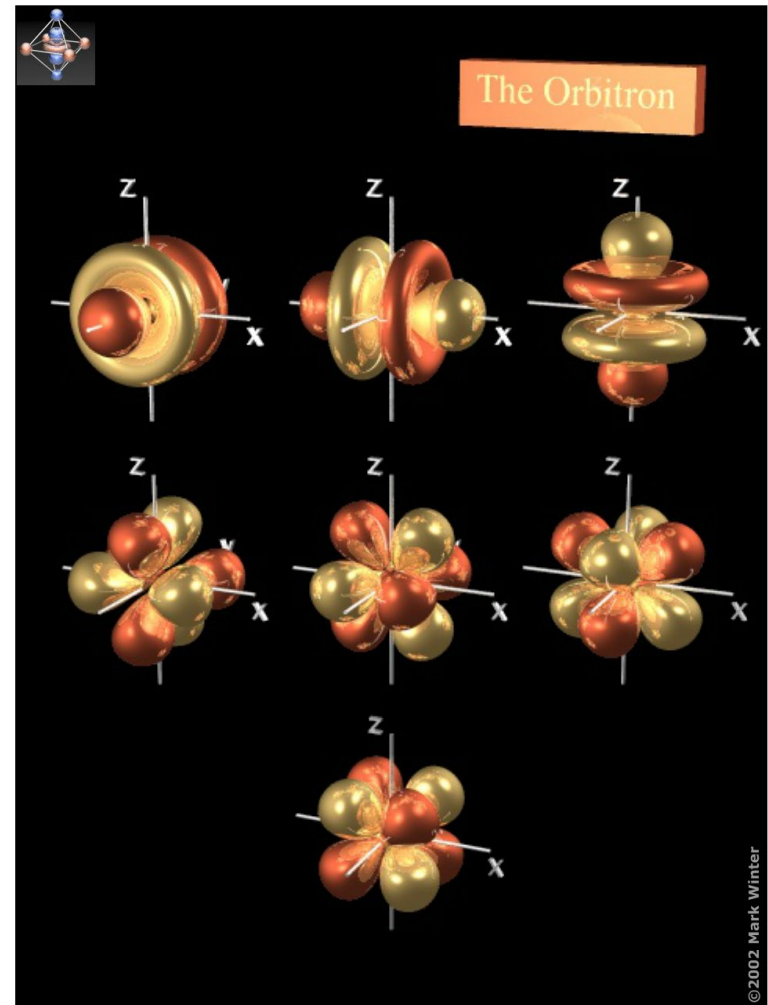


(c)



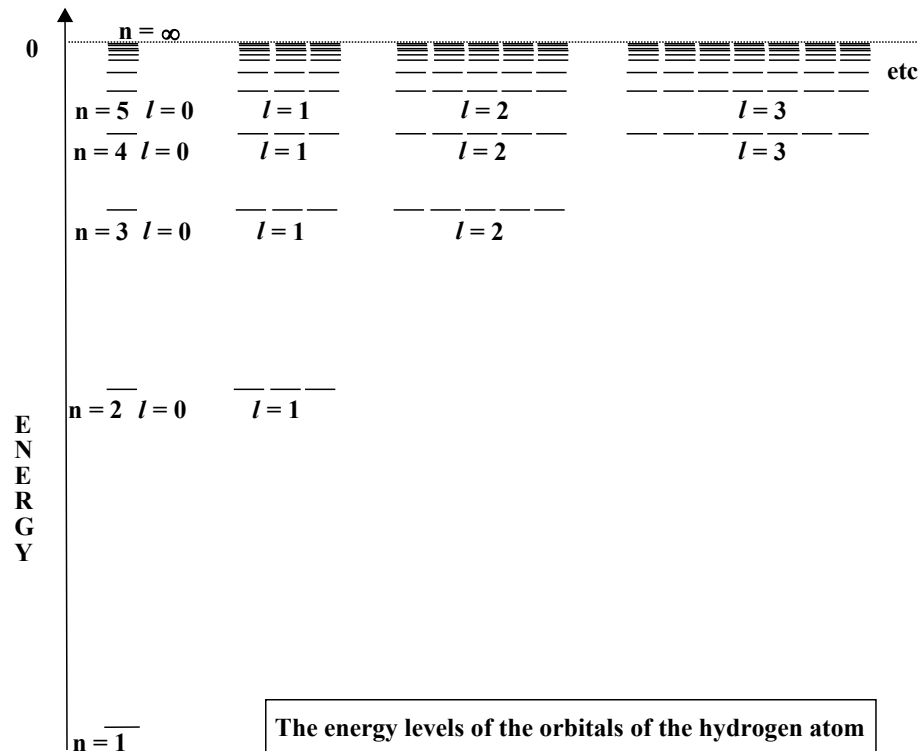
What do Orbitals Look Like?

- ***f* orbitals ($l = 3$)**
 - An *f* orbital has ___ planar nodes.
 - The higher *f* orbitals ($5f$, $6f$, etc.) also have radial nodes.
- When $l \geq 3$, orbitals become difficult for most people to draw. For pictures (probability surfaces) of orbitals with $l \geq 3$, see <http://winter.group.shef.ac.uk/orbitron/>



What do Orbitals Look Like?

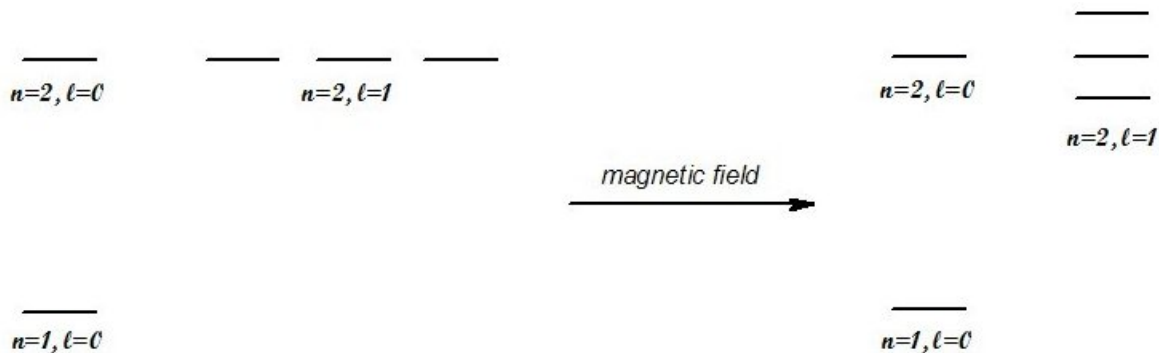
- An energy level diagram for the orbitals of a hydrogen atom according to the Schrödinger model:



- The energy of an orbital is given entirely by the principal quantum number (n), but there are many more orbitals present than the Bohr model predicts

What do Orbitals Look Like?

- If we zoom in on the lowest energy levels, we can see what would happen to them if we apply a magnetic field:



- The magnetic field interacts differently with different orbitals depending on their energy, shape and orientation. This changes the energy of some orbitals more than others, creating new energy levels. This is known as the **Zeeman effect**.
- Why is this relevant to atomic structure?