Name ________________________________**Chem 162, Section**: _______**Team Number:** ______

ALE 4. The Quantum Mechanical Model of the Hydrogen Atom

(Reference: Section 7.4 - *Silberberg 5th edition*)

What do the four quantum numbers tell us?

Quantum mechanics is a set of complex mathematics that is used to describe the most probable location of an electron outside the nucleus of an atom. Shortly after Neils Bohr proposed the planetary model of the atom, Werner Heisenberg proposed the ***Heisenberg Uncertainty Principle***, which stated that it is impossible to know both the exact position and the exact velocity of a small particle at the same time. The location of an electron in an atom is based on *probability*—the most likely location for an electron.

To locate the most probable location of a person you need 4 things. If you know 4 things: state, city, street and house number then you know the most probable location of the person. You also need 4 things, called "***quantum numbers***", to describe the most probable location for an electron

Table 1. The four quantum numbers and what they tell us

Quantum number	**What the Quantum number tells us**
Principal quantum number, n	which energy level the electron is in
Angular momentum quantum number, ℓ	which sublevel within the energy level the electron is in
Magnetic quantum number, m_ℓ	which orbital within the sublevel the electron is in
Spin quantum number, m_s	direction of electron spin (clockwise or counterclockwise)

The four quantum numbers—n, ℓ, m_ℓ and m_s—are solutions to a very complex equation, the ***Schrödinger equation***. The first three (n, ℓ and m_ℓ) describe the most probable location of an electron in 3-dimensional space—somewhat like how x, y, and z values describe the location of a point on a 3-dimensional graph. The last quantum number, the spin quantum number, m_s, tells us the direction an electron spins, clockwise or counterclockwise.

The Schrödinger equation in all its glory!

$$\frac{d^2\Psi}{dx^2} + \frac{d^2\Psi}{dy^2} + \frac{d^2\Psi}{dz^2} + \frac{8\pi^2 m_e}{h^2}(E - V(x,y,z))\Psi(x,y,z) = 0$$

wave function

mass of electron

potential energy at x,y,z

how ψ changes in space

total quantized energy of the atomic system

Table 2. Rules governing what values quantum numbers are allowed to have.

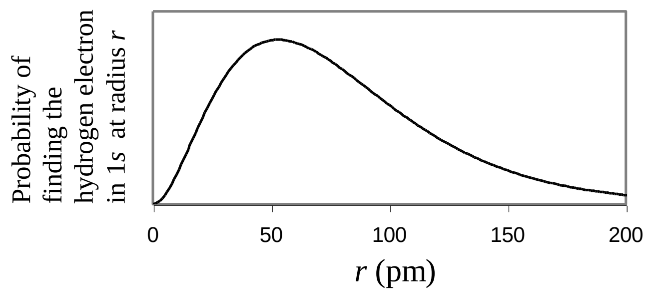
Quantum number	**Possible values**
n	1, 2, 3, 4, …integer values
ℓ	Integer values from 0 to n -1
m_ℓ	Intergers: - ℓ to + ℓ
m_s	+½ or -½

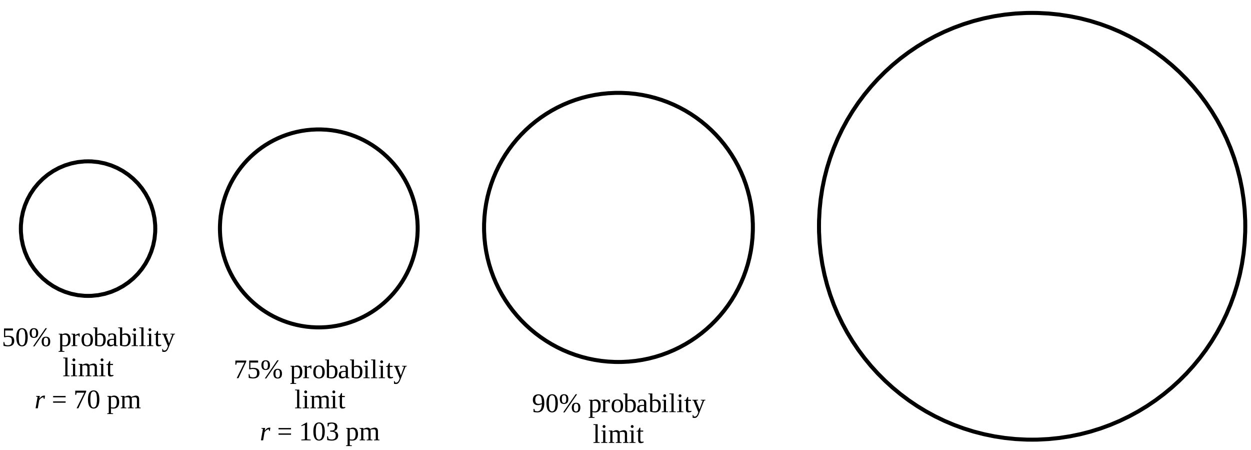
The models on the following pages will guide your understanding of the quantum numbers n, ℓ and m_ℓ.

The Model: Boundary Surface Diagrams

The ***Heisenberg Uncertainty Principle*** does not allow us to say that the electron can be found at a quantized distance from the nucleus (as is in the Bohr model of the hydrogen atom). Instead, the position of the electron can only be thought of in terms of the probability that an electron will be found within a certain distance of the nucleus.

An ***atomic orbital*** is a region of space around a nucleus that one is <u>*likely*</u> to find an electron. The lowest-energy orbital is the 1*s* (“one es”) orbital. The probability of finding an electron at various distances from the nucleus in the 1*s* orbital of the hydrogen atom is shown in the figure to the right. The ***boundary surface diagram*** of an orbital is a convenient way of sketching the orbital. The boundary surface diagrams of the hydrogen atom’s 1*s* orbital drawn at the 50%, 75%, 90%, and 99% probability limits are shown below. <u>*The tiny nucleus may be thought of as at the very center*</u>. <u>*The electron may be thought of as being ANYWHERE within a spherical region described by a certain radius from the central nucleus*</u>.





50% probability limit
r = 70 pm

75% probability limit
r = 103 pm

90% probability limit
r = 140 pm

99% probability limit
r = 222 pm

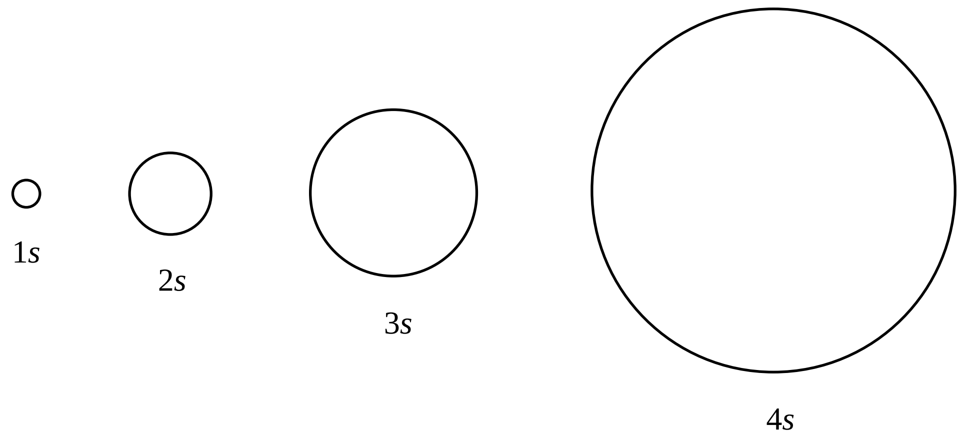
Key Questions

1. As the probability of finding an electron in an orbital increase, what happens to the way that the boundary surface diagram of the orbital is drawn?

2. Is it possible to draw a boundary surface diagram of the 1*s* orbital at the 100% probability limit? If it is, draw it relative to the boundary surface diagrams drawn at the 50%, 75%, 90%, and 99% probability limits. If it is not, explain why it is not.

The Model: The Principal Quantum Number

The hydrogen atom has a number of orbitals that can be described as being "*s* orbitals". They are the 1*s*, the 2*s*, the 3*s*, and so on. The first four *s* orbitals are drawn to scale below (each at the 90% probability limit).



Again, the electron is thought to exist SOMEWHERE within the region of space described by the above shapes (all spherical with respect to the central nucleus). The difference in the orbitals' names is the number in front of the *s*. That number is ***n***, the ***principal quantum number***. The principal quantum number may be any counting number (*i.e.*, $1 \leq n < \infty$). The relative energies of an electron in the *s* orbitals is ordered as follows: 1*s* < 2*s* < 3*s* < · · ·.

Key Questions

3. In the Bohr model of the hydrogen atom how are the distance of an electron from the nucleus and the energy of an electron related to the principal quantum number *n*?

4. As it pertains to the distance an electron spends away from the nucleus, the value of *n* is somewhat different in the Bohr model than in the quantum mechanical model. Describe this difference. (Keep in mind that the quantum mechanical model subscribes to the Heisenberg Uncertainty Principle.)

The Model: The Angular Momentum Quantum Number, ℓ

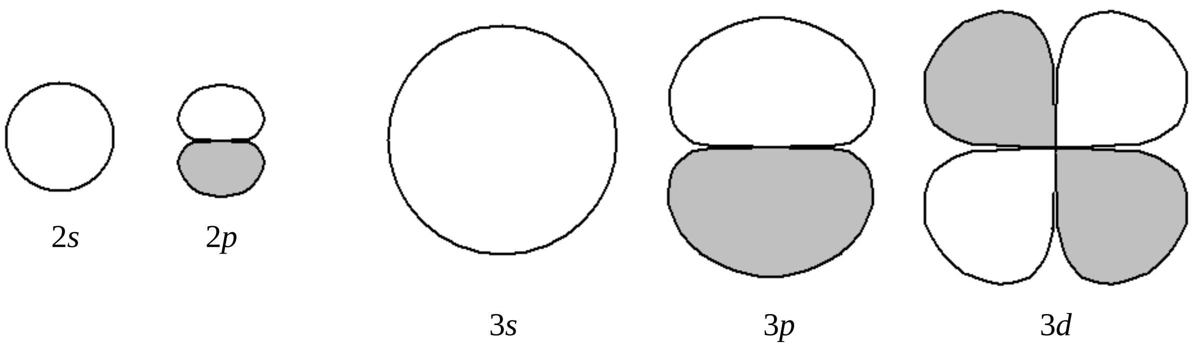
The ***angular momentum quantum number***, $\boldsymbol{\ell}$, describes the shape of the region of space in which an electron may be found. The numerical value of ℓ of an electron determines the type of orbital the electron is in.

ℓ	**orbital**
0	*s*
1	*p*
2	*d*
3	*f*

The value of the principal quantum number dictates what values that the angular momentum quantum number may have. Given that the value of the principal quantum number for an energy level) is *n*, then **the allowed values of the angular momentum quantum number for orbitals within that energy level are all possible integers (whole numbers) between (and including) 0 and *n* – 1:**

$$\boldsymbol{\ell = 0 \text{ to } n - 1}$$

For example, when the electron of the hydrogen atom is promoted from the first shell (*i.e.*, $n = 1$) to the second energy level (*i.e.*, $n = 2$), not only may the electron be found in the 2*s* orbital, but the electron may also be found in a 2*p* orbital.



When the electron is promoted to the third shell, the electron may be found in either the 3*s* orbital or a 3*p* orbital or a 3*d* orbital. (*<u>All orbitals are drawn to scale in the above figures</u>*.)

Key Questions

5a. What is the shape that all *s* orbitals have?

b. What is the shape that all *p* orbitals have?

c. What is the primary difference between a 2*p* and a 3*p* orbital?

d. Sketch a 3*d* orbital and next to it sketch a 4*d* orbital. Label the orbitals so the reader will know which is which.

6. A nodal plane is a plane on which it is impossible to find an electron.
   a. Show with a drawing how the shape of a *p* orbital is formed when a nodal plane is passed through the middle of an *s* orbital.

   b. Draw a sketch that might describe what an *f* orbital looks like. ***Hint***: Just as a nodal plane bisects an S orbital to form a P orbital, a nodal plane passes down a *p* orbital to create a *d* orbital. Use this information to draw a sketch that might describe what an *f* orbital looks like.

7. Use quantum numbers to determine the first energy level (*i.e.*, what is the minimum value of *n*) that contains an *f* orbital?

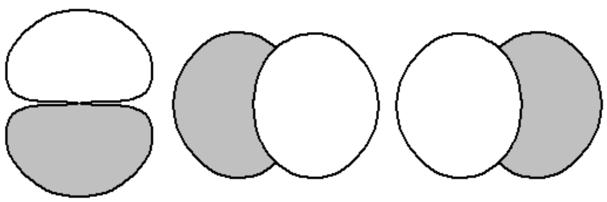
8. There no such thing as a 1*p* or a 2*d* orbital. *Use quantum numbers to explain why*.

The Model: The Magnetic Quantum Number, m_ℓ

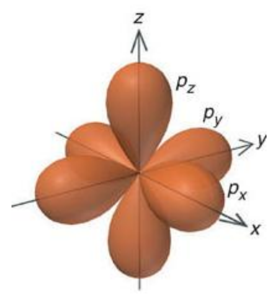
Within an energy level (identified by the value of n) there will be one or more sublevels (identified by the value of ℓ). The ***magnetic quantum number***, $\boldsymbol{m_\ell}$, distinguishes from each other orbitals that are within the same sublevel. Different orbitals within the same sublevel will have the same value of ℓ but different values of m_ℓ – they all have the same shape, but are pointing differently in space relative to each other. Given that the value of the angular momentum quantum number is ℓ, then **the allowed values of the magnetic quantum number for orbitals within that sublevel are all possible integers between and including -ℓ and +ℓ**:

$$m_\ell = -\ell \text{ to } +\ell$$

Within the $3p$ sublevel, there are the $3p_x$, $3p_y$, and $3p_z$ orbitals, named such because they are perpendicular to each other and can be thought to lie on the x-, y-, and z-axes of Cartesian space.



$3p_z$ $3p_y$ $3p_x$



Key Questions

9a. What is the value of ℓ for an electron in a p orbital?

b. Given that value of ℓ in Question 9a, what are the allowed values of m_ℓ for a p sublevel?

c. How many allowed values of m_ℓ are there? Compare this number to the number of p orbitals in the $3p$ sublevel in the Model. *Show your work using quantum numbers.*

10a. What are the allowed values of m_ℓ for a d sublevel? *Show your work using quantum numbers.*

b. How many d orbitals are in a d sublevel? *Show your work using quantum numbers.*

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11. Fill in the blanks in the following two tables.

Table 3.

Principle Quantum Number (n)	**Sublevels that are possible**	**Possible values for ℓ**
n = 1		
n = 2	s and p	0 or 1
n = 3		0, 1, or 2
n = 4	s, p, d and f	

Table 4.

Angular momentum Quantum number, ℓ	Sublevel	# of Orbitals Possible in the sublevel	Possible m_l values
0	s	1	0
1			
2			
3			

12. Problem 7.50: How many *__orbitals__* in an atom can have each of the following designations? *__Use quantum numbers to explain/show how you arrive at each of your answers__*.

a.) 5 *f*

b.) 4*p*

c.) 5*d*

d.) $n = 2$

13. Given the quantum numbers (n, ℓ, m_ℓ and m_s), which of the following combinations are NOT possible. (There may be more than one.) *__Explain.__*

a) (3, 3, 2, -1/2) b) (4, 1, -1, +1/2) c) (0, 0, 0, -1/2) d) (2, 1, -1, +1/2)