Chapter 7 - Quantum Model of Atom

Section 3 – Quantum Numbers

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Introduction

Quantum theory gave scientists an idea of shells in atoms where electrons can be found. These shells are designated by the letter “n”. Giving energy to atoms will cause electrons to go from a lower energy level of n (shell) to a higher n level. Energy is given off when these electrons come back to their ground level.

In this section we are going to learn exactly where the electrons are in the shell in an atom. Each electron has its own location and how and where it moves in that space. These spaces are determined by quantum numbers.

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Quantum Numbers

According to quantum theory, each electron is described by four quantum numbers:

1. Principal quantum number (*n*)
2. Angular momentum quantum number (*l*)
3. Magnetic quantum number (m_l)
4. Electron spin quantum number (m_s)

The first three define the wave function for a particular electron. The fourth quantum number refers to the magnetic property of electrons.

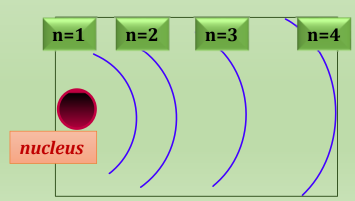
A wave function for an electron in an atom is called an atomic orbital (described by three quantum numbers—*n*, *l*, m_l). It describes a region of space with a definite shape where there is a high probability of finding the electron.

Principal quantum number (n)

***Principal quantum number* (n)** designates size of the orbit or shell. This is the first number in the quantum numbers. Electrons exist in these shells.

- **n numbers have integer values** 1,2,3, and so forth.

  n numbers cannot be a fraction, negative or zero.
- The larger the "n" value, the greater the average distance from the nucleus and the greater the size of the orbit/shell.
- As the distance from the nucleus increase, the energy of that shell also increases.
- Keep in mind that the distance between the shells, in blue curves shown below, may not be equal.



Angular momentum quantum number (*l*)

Angular momentum quantum number **(*l*)** – This designates the shape of the atomic orbital or subshell. Remember that electrons themselves are all the same particles. This shape here represents the "space" where there is a probability of finding an electron.

l integer values can be calculated as **n**-1, with values all number **n**-1 to 0. 0 to $n - 1$.

When **n = 1**, then *l* = 1-1 = 0

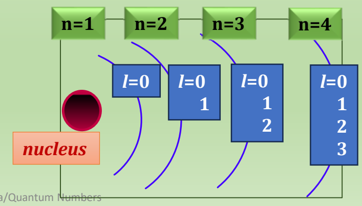
When **n = 2**, then *l* = 2-1 = 0, 1

When **n = 3**, then *l* = 3-1 = 0, 1, 2

What this means is that in shell n = 1, only one space, 0, for electrons exist. When n = 2 then there are two subshells, 0 and 1, exist; that is, there two spaces for electrons to exist.

Values of *l* can be zero and not negative. As the shell number increase the numbers of *l* values also increase. These *l* values are assigned alphabets.

l = 0 = *s subshell; shape is spherical*
l = 1 = *p subshell; shape is dumbbell*
l = 2 = *d subshell; various shapes*
l = 3 = *f subshell; various shapes*



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Magnetic quantum number (m_l)

Magnetic quantum number **(m_l)** – This is the orientation of the orbital/subshell in space. Here you should think in terms of three dimensions (*x*, *y* and *z* axes). This number indicates the space where the electron is moving within the subshell in the shell.

Integer values: – *l* to 0 to + *l*

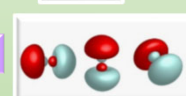
s When *l* = 0; m_l = 0. This indicates one orientation in space. *l* has a spherical shape; so m_l is only one kind – spherical.

p When *l* = 1; m_l = -1, 0, +1. *l* = 1 is dumbbell shape; the +1, 0 and -1 indicate the dumbbells are in three different directions (x, y and z).

d When *l* = 2; m_l = -2, -1, 0, +1, +2. There are 5 orientations.

f When *l* = 3; m_l = +3, +2, +1, 0, -1, -2, -3. There are 7 orientations.

s


p


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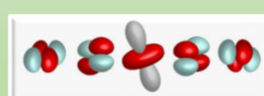

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Magnetic quantum number (m_l)

There are 2 electrons (e⁻) in each orientation, hence m_l = 0 has 2 e^-. The table below shows the number of electrons possible in each orientation.

When l	m_l	Shape	Orientations	No. of e^-
l = 0	0	Spherical	1	2
l = 1	-1, 0, +1	Dumbbell	3	6
l = 2	-2, -1, 0, +1, +2	Various	5	10
l = 3	+3, +2, +1, 0, -1, -2, -3	Various	7	14

See the next slide to see how we can use this information to see an overview of an atom with four shells. We can understand how many electrons exist in each shell and which orientations.

The electrons in these shells are always in motion around the nucleus and within the orientations in wave form.

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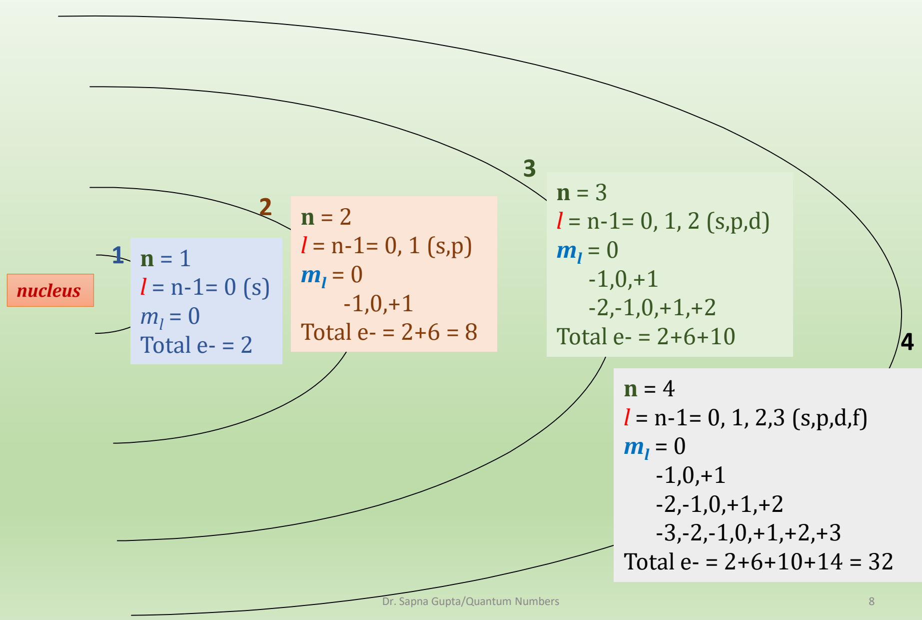
Atomic View of Quantum Numbers



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Electron spin quantum number (m_s)

Electron spin quantum number **(m_s)** – This is the last of the quantum numbers. It determines the spin of an electron that occupies a particular orbital/subshell in one orientation.

- **Values**: +1/2 or –1/2. These numbers are independent of all the other quantum numbers.
- Just like electrons are in motion around the nucleus in wave form, they are also in motion in each of the orientations they occupy (**m_l** number). This spinning is akin to the earth spinning in its own axis generating a magnetic field. For this this reason two electrons cannot spin in the same direction in the individual orientations.
- This quantum numbers indicates that electrons will spin opposite each other in the same orbital.

Quantum Numbers - Summary

	Principal quantum number	***Angular momentum quantum number***	***Magnetic quantum number***	***Electron spin quantum number***
Alphabet	n	*l*	m_l	m_s
What it does	Designates size of the orbit/shell.	Gives the shape of the atomic orbital/subshell.	It is the orientation of the orbital/subshell in space (3D orientation).	This is the spin of an electron in an orbital/subshell.
How to Calculate	Integer values: 1,2,3, and so forth	Integer values: 0 to *n* – 1	Integer values: – *l* to 0 to + *l*	Values: +1/2 or –1/2
Other information	The larger the "*n*" value, the greater the distance from the nucleus. Energy increases with n number.	0 = *s shape/orbital* 1 = *p shape/orbital* 2 = *d shape/orbital* 3 = *f shape/orbital* Energy increases with ***l*** number.	There are 2e- in each orientation. All orientations are degenerate (equal energy)	Electrons spin opposite each other in the same orbital at ground state.

Quantum Numbers – Allowed numbers

	Allowed Values		
When n is	*l* can be	When *l* is ->	m_l can be
1	**0**	**0**	**Only 0**
2	**0 and** **1**	**0** **1**	**Only 0** **-1, 0, +1**
3	**0,** **1 and** **2**	**0** **1** **2**	**Only 0** **-1, 0, +1** **-2, -1, 0, +1, +2**
4	**0,** **1,** **2 and** **3**	**0** **1** **2** **3**	**Only 0** **-1, 0, +1** **-2, -1, 0, +1, +2** **-3, -2, -1, 0, +1, +2, +3**

Understanding Quantum Numbers

•**When *n* = 1, *l* has only one value, 0.**

•When ***l*** = 0, m_l has only one value, 0.

Thus, the first shell (*n* = 1) has one subshell, an *s*-subshell, 1*s.* That subshell, in turn, has one orbital with capacity of $2e^-$.

•**When *n* = 2, *l* has two values, 0 and 1.**

•When ***l*** = 0, m_l has only one value, 0. So there is a 2*s* subshell with one orbital of $2e^-$ capacity.

•When ***l*** = 1, m_l has only three values, -1, 0, 1. So there is a 2*p* subshell with three orientations and $6e^-$ capacity.

•**When *n* = 3, *l* has three values, 0, 1, and 2.**

•When ***l*** = 0, m_l has only one value, 0. So there is a 3*s* subshell with one orbital of $2e^-$ capacity.

•When ***l*** = 1, m_l has only three values, -1, 0, 1. So there is a 3*p* subshell with three orientations and $6e^-$ capacity.

•When ***l*** = 2, m_l has only five values, -2, -1, 0, 1, 2. So there is a 3*d* subshell with five orientations and $10e^-$ capacity.

Solved Problem: Determining if quantum numbers are permitted

Which of the following are permissible sets of quantum numbers?

n = 3, l = 4, m_l = 0, m_s = ½
n = 3, l = 2, m_l = 0, m_s = -½
n = 2, l = 0, m_l = 0, m_s = - $^3/_2$
n = 5, l = 4, m_l = -3, m_s = ½

(a) Not permitted. When n = 3, the l = 4 is not possible since l = n -1

(b) Permitted.

(c) Not permitted; m_s can only be +½ or –½.

(b) Permitted.

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Solved Problem: Determining quantum numbers of electrons

What are the quantum numbers of the following electrons?

a) 3p
b) 5d
c) 6s

(a) n = 3, l = 1, m_l = 0, m_s = ½

n = 3, l = 1, m_l = Can be +1, 0 or -1, m_s = can be + ½ or -½

(b) n = 5, l = 2, m_l = 0, m_s = -½

n = 5, l = 2, m_l = Can be +2,+1, 0, -1 or -2 m_s = can be + ½ or -½

(c) n = 0, l = 0, m_l = 0, m_s = ½

n = 0, l = 0, m_l = can only be 0, m_s = can be + ½ or -½

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Final Thoughts on Quantum Numbers

- What quantum numbers tell us is what numbers are allowed and which are not by the formulas given. This indicates that electrons don't just randomly occupy spaces in an atom.
- We will learn later how electrons are filled in each shell in a systematic and logical order.
- As the shell number increases, the size of the shell increases. The size of the orbitals also increases. The next few slides show how the size of these orbitals increase with shell numbers.

s - orbital

The blue-green cross-sectional view of a 1*s* orbital and a 2*s* orbital highlights the difference in the two orbitals' sizes.

The larger sizes of the s orbitals show a better sense of them in three dimensions.

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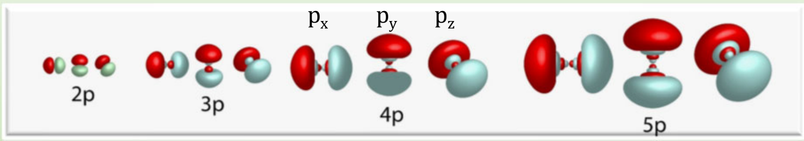
p and d orbitals

A *p* orbital has two lobes along a straight line through the nucleus, with one lobe on either side. There are three orientations. The size of the subshell increases as the n number increases.



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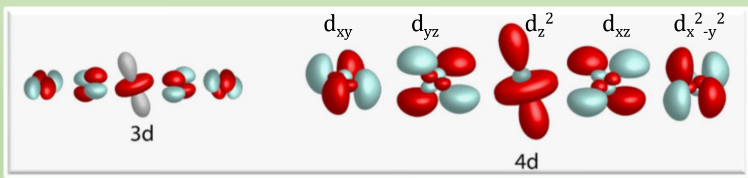
A *d* orbital has shapes based on four lobes and has five orientations. *d* orbitals start from shell number 3.



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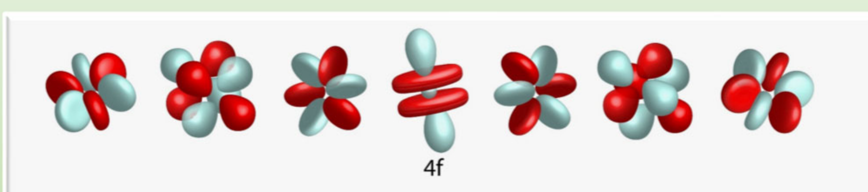
F-orbitals

f orbitals are more complicated than *d* and have seven orientations. *f* orbitals start from shell number 4.



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All orbitals – 4th Shell – 32 electrons

2 e-

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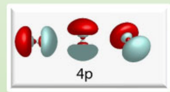

6 e-

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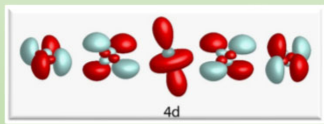

10 e-

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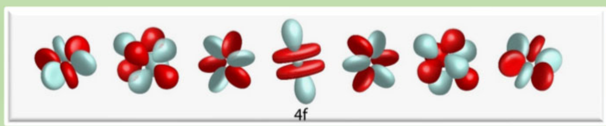

14 e-

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Key Points

- Quantum numbers (n, l, m_l, m_s) predict values and possible sets.
- Shapes of orbitals.