Department of Mathematics and Natural Sciences

CHE 101: Introduction to Chemistry

Lecturer: ***Muhammad Mahfuz Hasan***

Lecture- 03

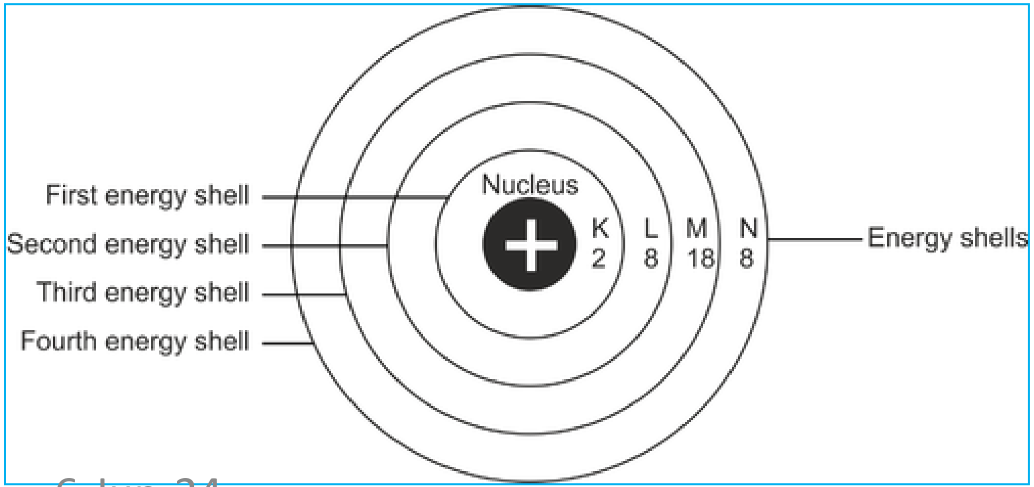
Content: Different quantum numbers, Orbit and Orbital, Electronic configurations

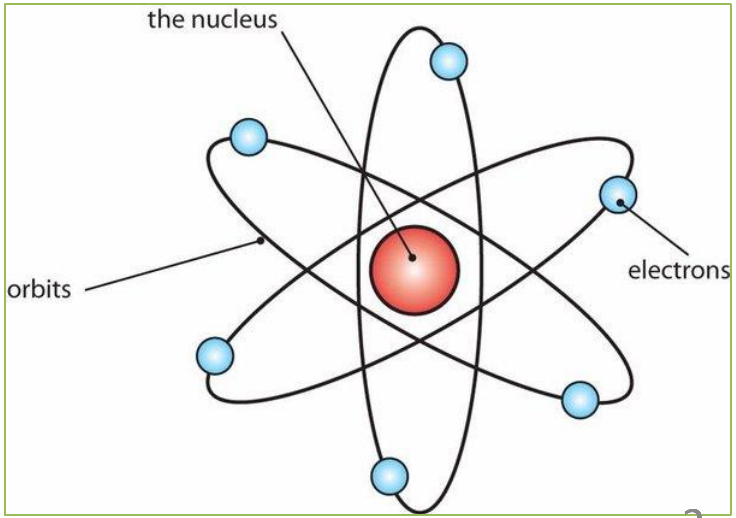
Orbit and Orbital

In an atom electrons move around the nucleus in a two dimensional, spherical fixed energy levels which is called the orbit.

The orbit nearest to the nucleus is the first energy level and is called **‘K shell’.** The next orbits are named as **L, M, N and so on.**

The three dimensional region in space around the nucleus where the probability of finding an electron is maximum (90-95 %) is called **orbital.**





Difference between orbit and orbital

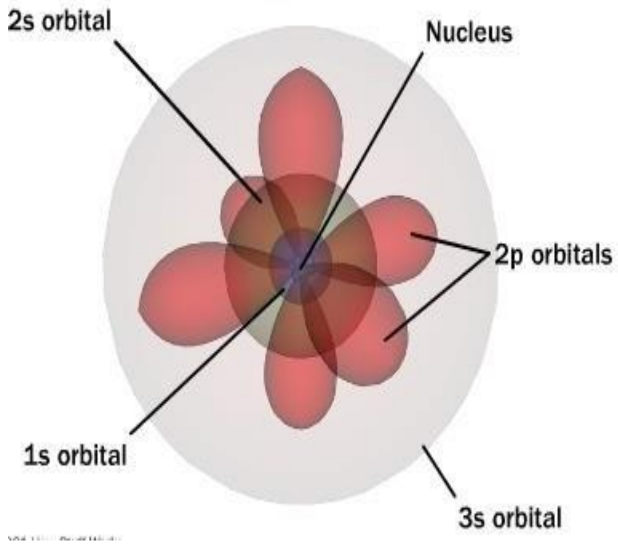
Orbit	Orbital
Orbits are definite path or energy level followed by an electron, according to Bohr	The three dimensional region in space around the nucleus where the probability of finding an electron is maximum (90-95 %) is called **orbital.**
It is represented two dimensionally.	An orbital is three dimensional representation.
The orbits may be circular or elliptical.	Different orbitals have different shapes. e.g. s orbital spherical, p orbital dumbbell shaped
Two orbits in an atom cannot have the same energy.	Two orbitals can have the same energy e.g., p_x p_y, p_z have the same energy.
An orbit can hold $2n^2$ number of electrons where n is the principle quantum number having the values 1, 2, 3 etc.	Each orbital can hold maximum two electrons of opposite spin e.g. s orbital holds 2, three p orbitals hold 6 and 5d orbitals hold 10 electrons.

Different types of orbitals

There are four types of orbital: s, p, d and f

1) **s-orbital** is **spherical** shaped with nucleus at the center

2) **p-orbital** is **dumbbell shaped**



❖ It's divided into three orbital with same energy

❖ They are p_x p_y, p_z

❖ They lie on x, y and z axis perpendicular to each other

3) **d-orbital** - there are **five** different orbitals

4) **f-orbital** - there are **seven** f orbitals

Orbitals

Orbitals

Each sublevel (s, p, d, f) contains orbitals.

Remember, orbitals are electron-clouds that hold the electrons 90% of the time.

Each orbital can hold TWO electrons, so

- s - 2 electrons, 1 orbital
- p – 6 electrons, 3 orbitals
- d – 10 electrons, 5 orbitals
- f – 14 electrons, 7 orbitals

Quantum Numbers

- **Quantum numbers** are a set of values that describes the state of an electron including the size of an electron orbit (energy levels), the shape of the orbitals, orientation of orbital in the magnetic field and the spin of electrons about its own axis.
- A number which occurs in the theoretical expression for the value of some quantized property of a subatomic particle, atom, or molecule.
- **The set of numbers used to describe the position and energy of the electron in an atom** are called quantum numbers.

Quantum Numbers

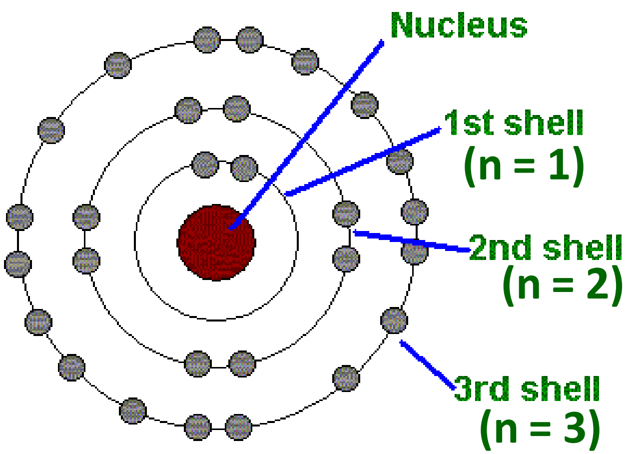
The above four characteristics are represented by four Quantum Numbers

i. Principal quantum number (n)
ii. Azimuthal or subsidiary quantum number (l)
iii. Magnetic quantum number (m_l)
iv. Spin quantum number (m_s)

i) Principal quantum number (n)

Express → Number of energy level

Indicates → size of orbit → distance of orbit from nucleus → Energy of electrons



Determine → total number of electrons in a shell (by $2n^2$)

Shells are designated by letters also →

K	L	M	N …..
1	2	3	4 …..

ii) Azimuthal quantum number (*l*)

Express → Concepts of orbitals of **different shapes**

possible values of *l* → **0 to (n-1)**
e.g. n = 3, l = 0, 1, 2

Indicates → shapes and numbers of orbitals in a shell

Determine → total number of electrons in an orbital as $2(2l+1)$

Subshells are denoted by letters as →

Letter	s	p	d	f	g …
l	0	1	2	3	4 …

Maximum number of electrons → 2, 6, 10, 14

iii) Magnetic quantum number (m_l)

indicates → orientation of orbitals in 3 dimensional space

allowed values → - *l* through 0 to + *l*

For $l = 0$, $m_l = 0$ (s subshell)

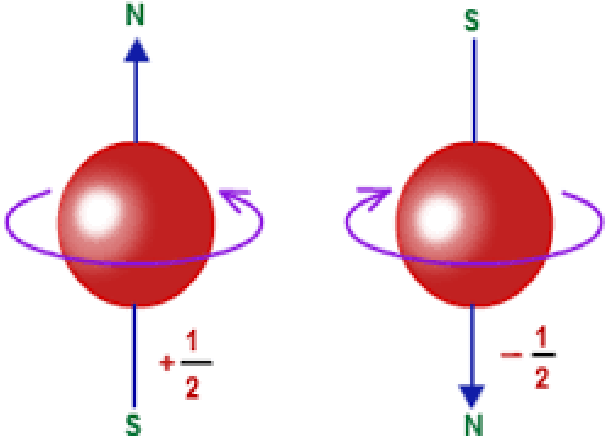
For $l = 1$, $m_l = -1, 0, +1$ (p subshell)

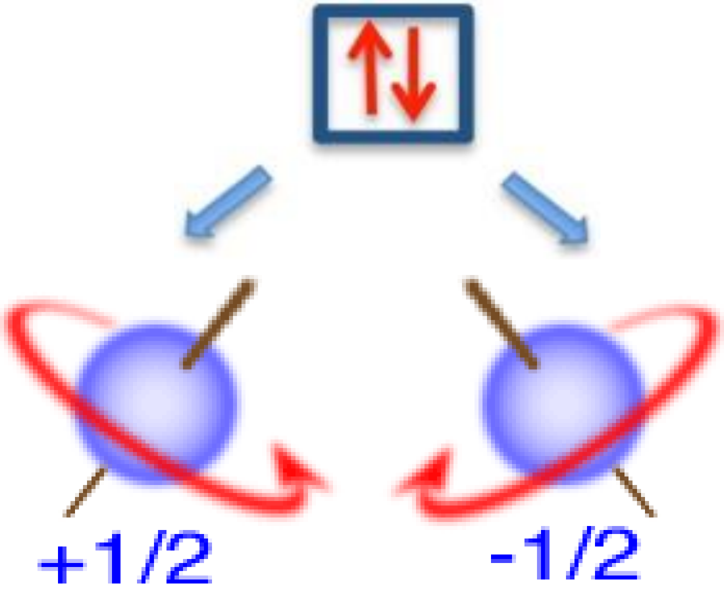
Determine → total number of orbital in a **subshell**

iii) Spin quantum number (m_s)

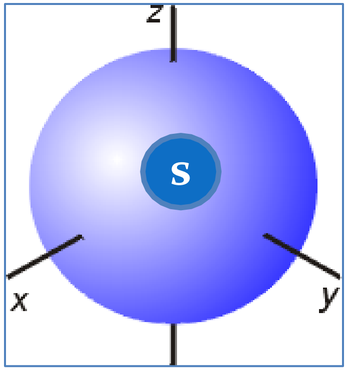
indicates → Two possible orientation of the spin axis of an electron

possible values → +1/2 or -1/2 for each value of m

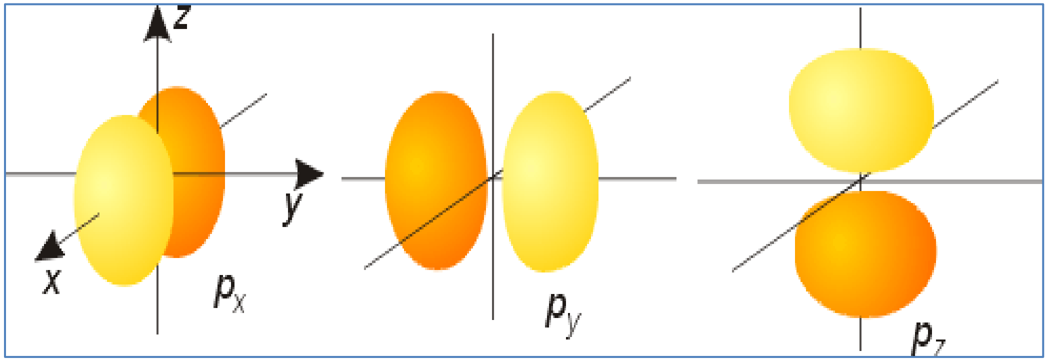


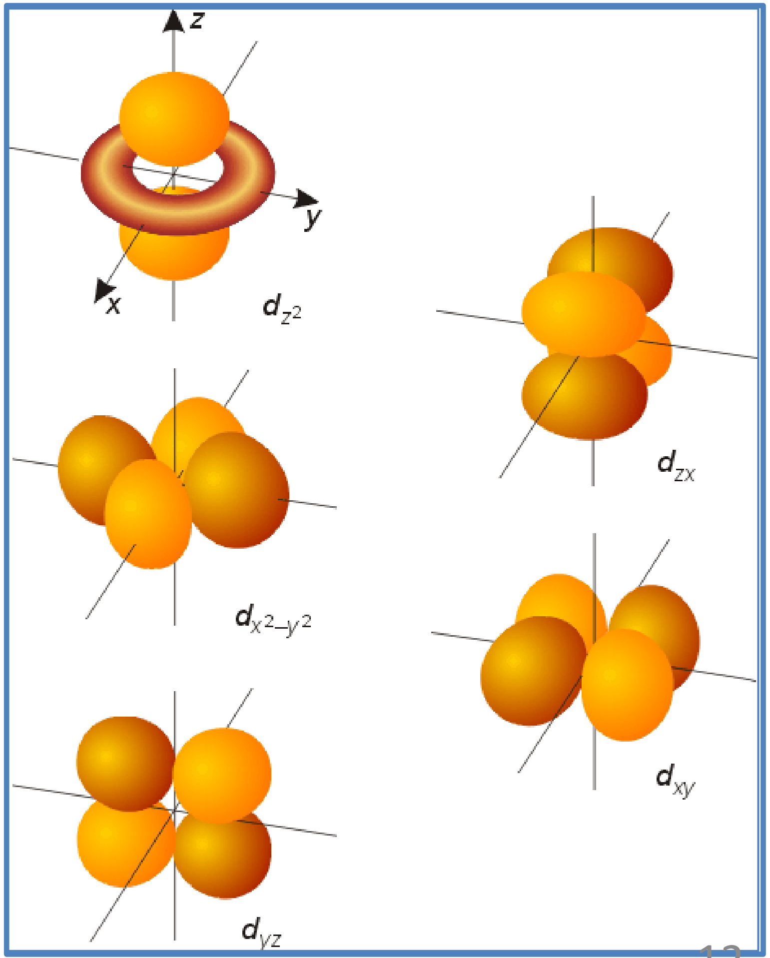


Different types of orbital with different quantum numbers



l =0,



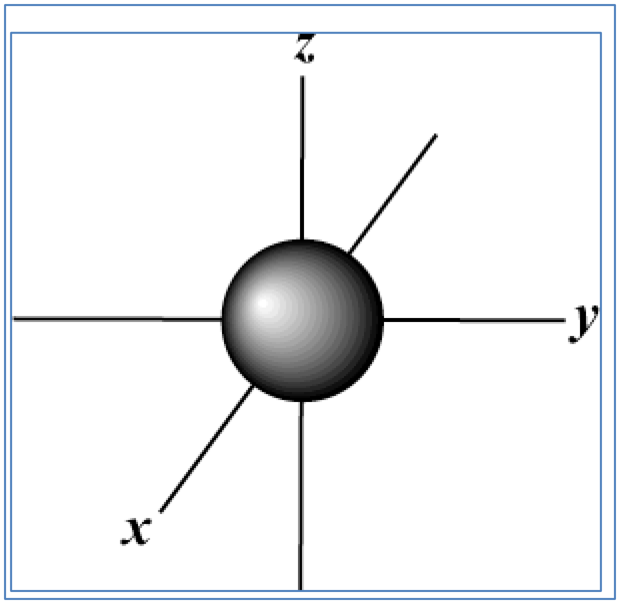


l =1, m=-

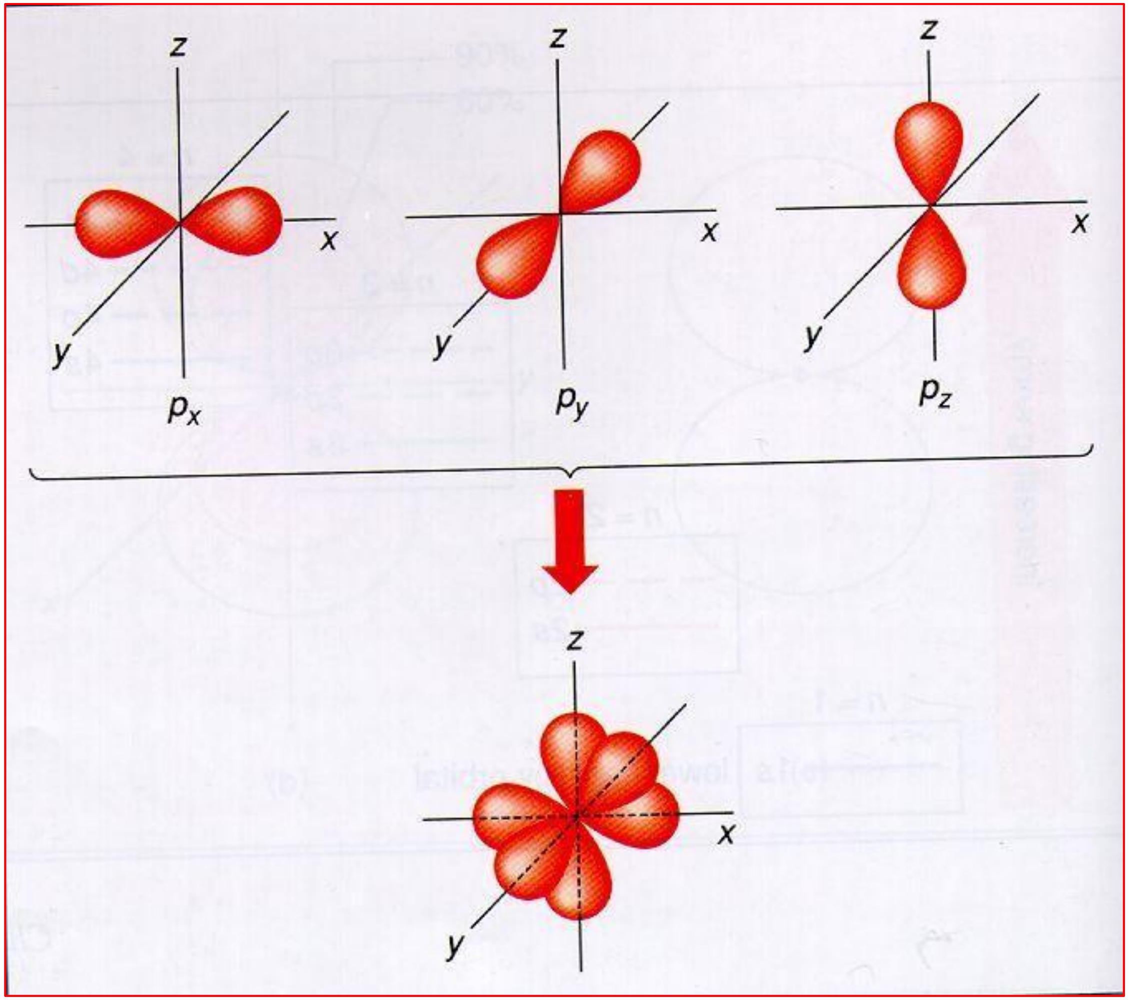
l=1, m=0

l=1, m=+1

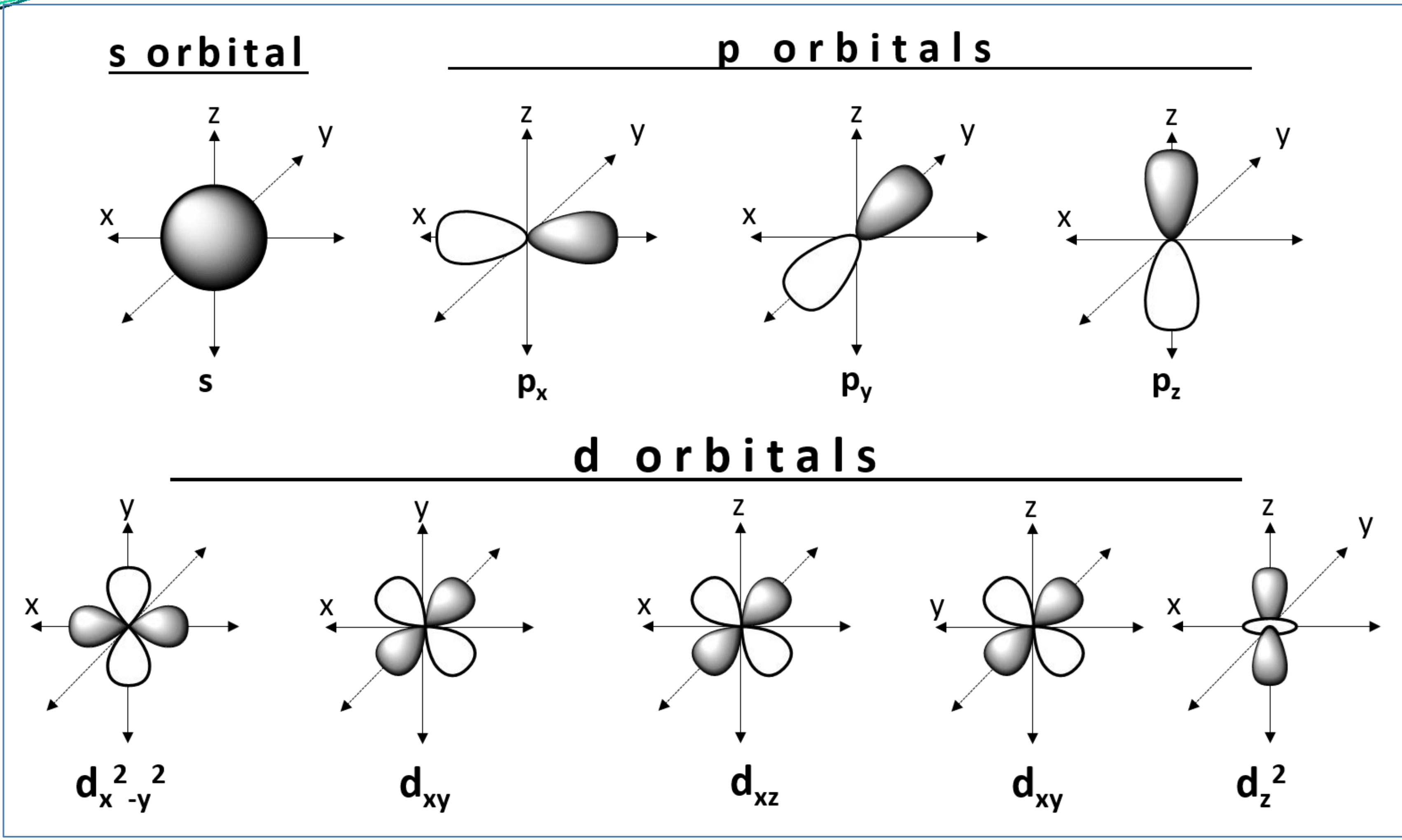
Shapes of different types of orbital



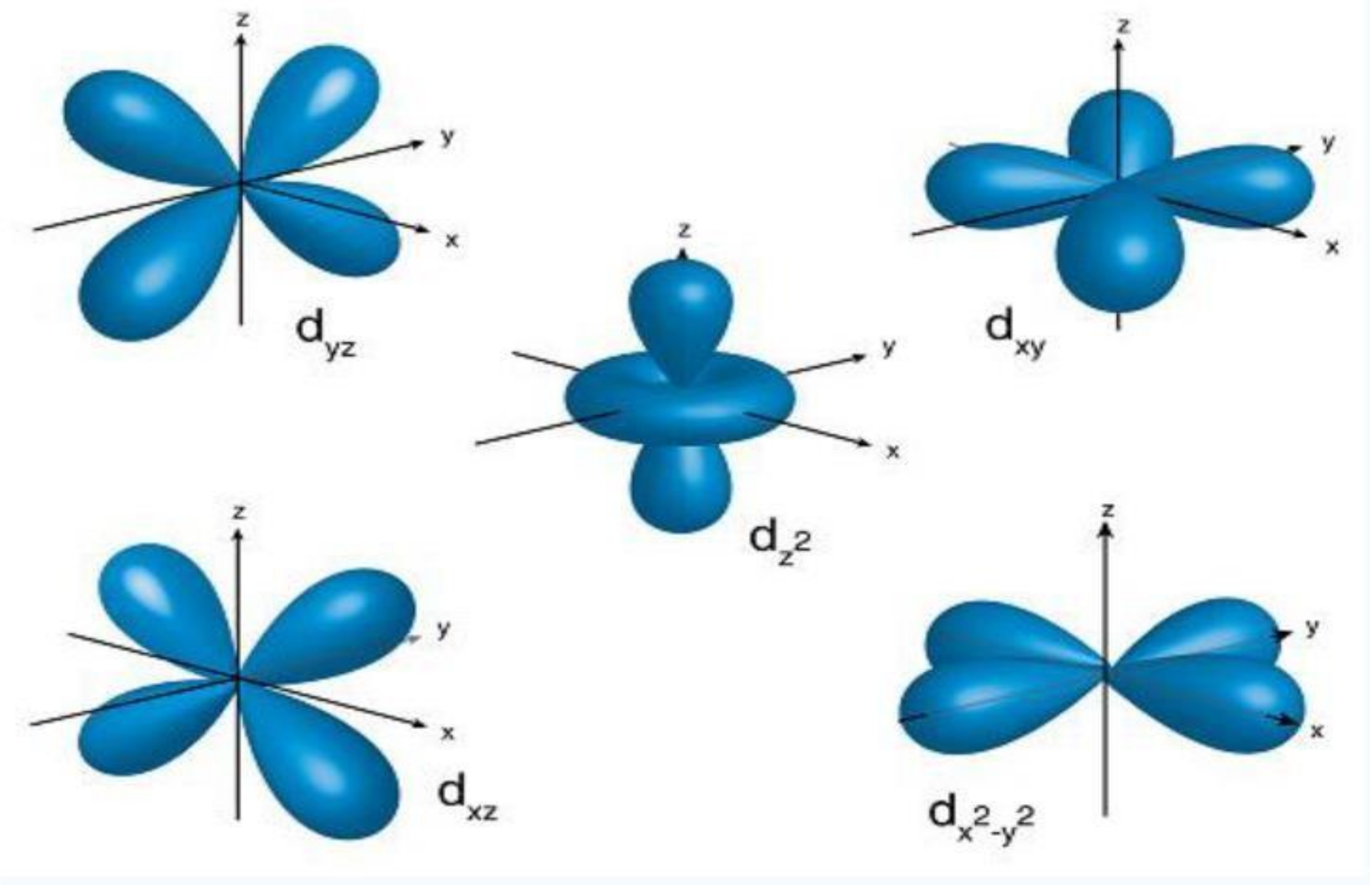
s-orbital
(spherical shape)



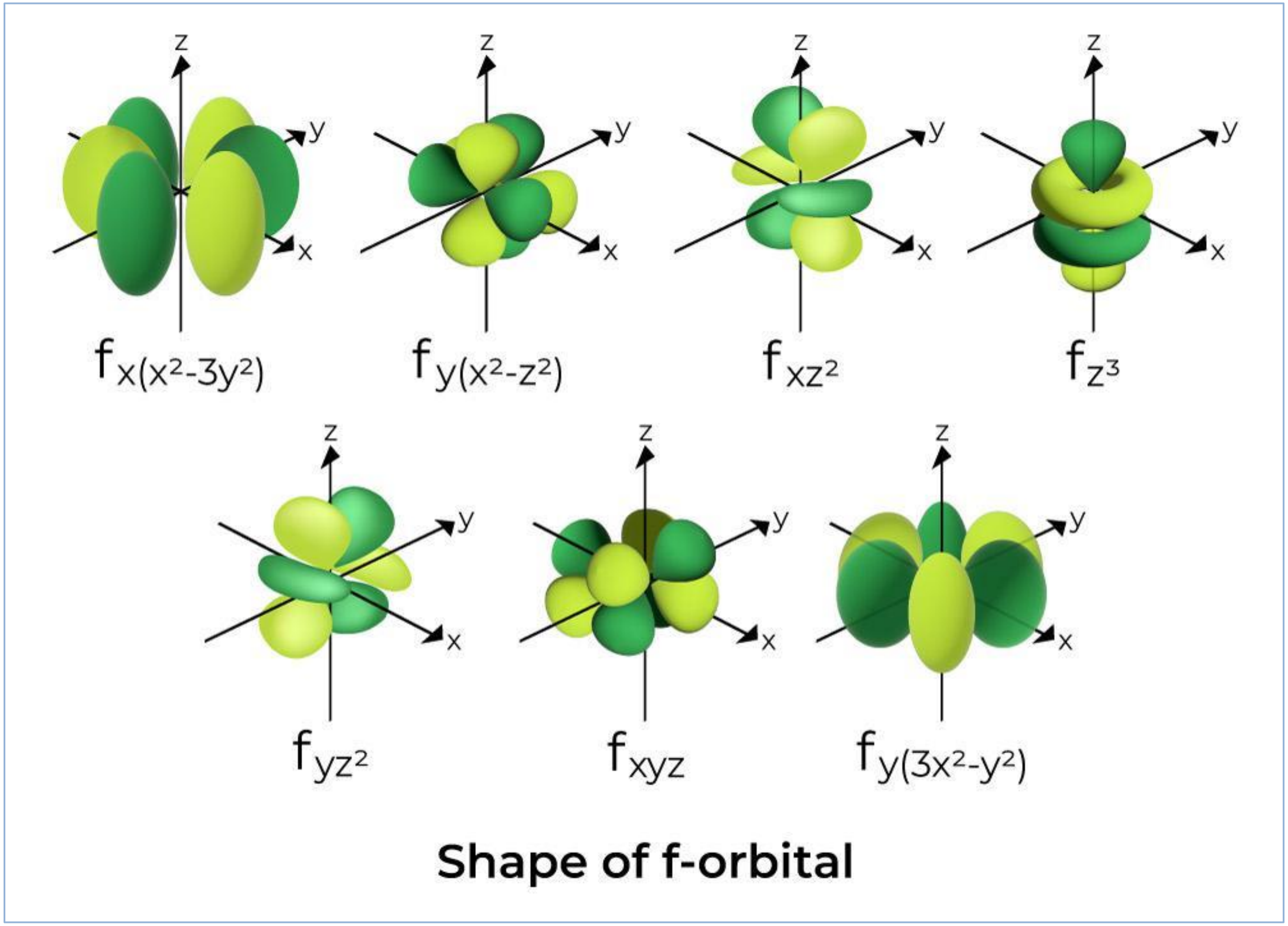
p-orbitals (dumbbell shaped)


s orbital
p orbitals
s
p_x
p_y
p_z
d orbitals
d_x2-y2
d_xy
d_xz
d_xy
d_z2

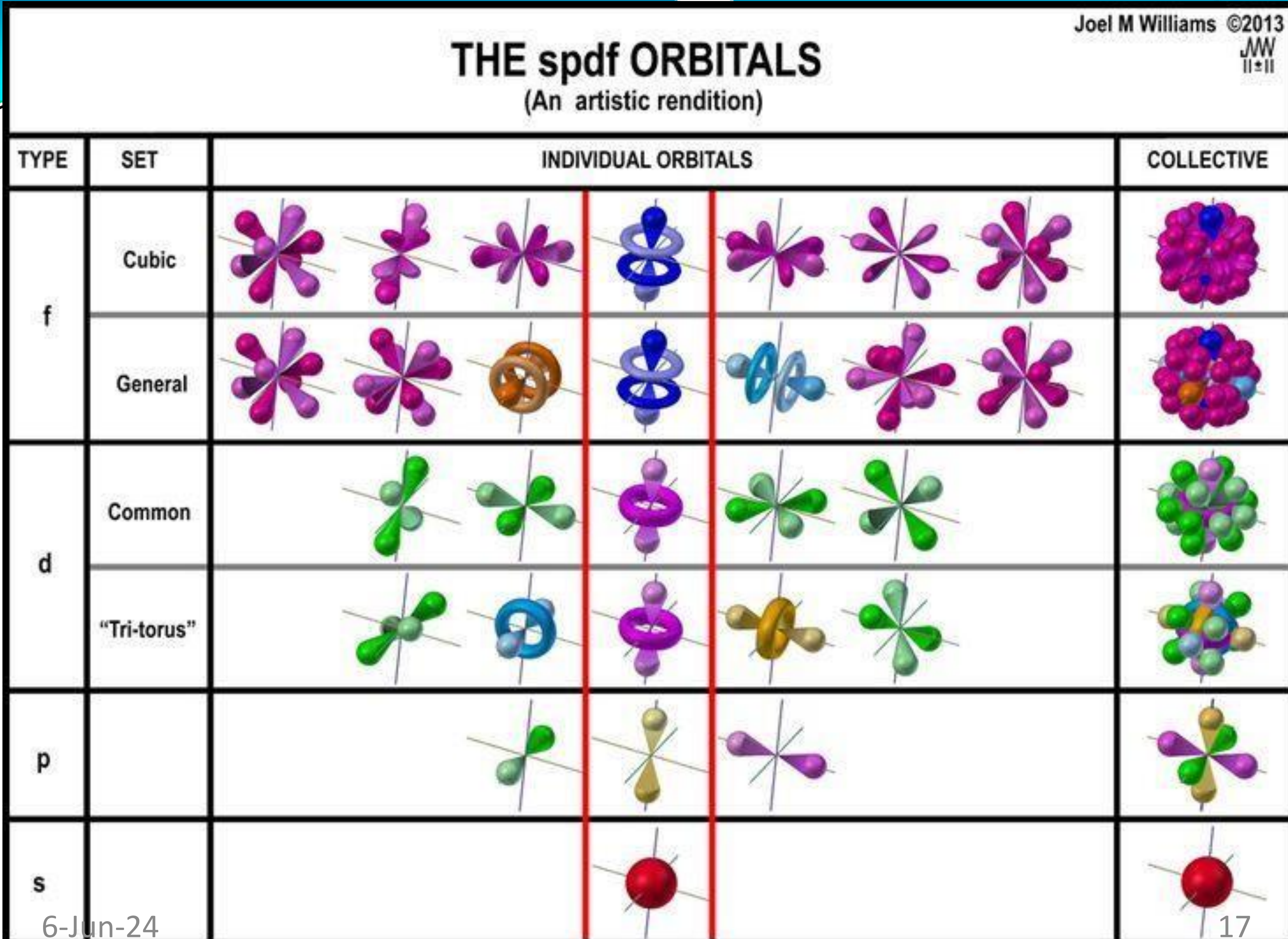
Shapes of d-orbital (3d)



F-Orbitals!



If you want to see more, go to:
http://www.orbitals.com/orb/orbtable.htm


Joel M Williams ©2013
THE spdf ORBITALS
(An artistic rendition)
TYPE
SET
INDIVIDUAL ORBITALS
COLLECTIVE
f
Cubic
General
d
Common
“Tri-torus”
p
s

Quantum Numbers

n	l	m_l	Orbital
$n = 1$	0	0	1*s*
$n = 2$	0	0	2*s*
	1	−1, 0, 1	2*p*
$n = 3$	0	0	3*s*
	1	−1, 0, 1	3*p*
	2	−2, −1, 0, 1, 2	3*d*
$n = 4$	0	0	4*s*
	1	−1, 0, 1	4*p*
	2	−2, −1, 0, 1, 2	4*d*
	3	−3, −2, −1, 0, 1, 2, 3	4*f*
$n = 5$	0	0	5*s*
	1	−1, 0, 1	5*p*
	2	−2, −1, 0, 1, 2	5*d*
	3	−3, −2, −1, 0, 1, 2, 3	5*f*
	4	−4, −3, −2, −1, 0, 1, 2, 3, 4	5*g*

Quantum Numbers

n	l	m_l	Orbital
$n = 6$	0	0	$6s$
	1	−1, 0, 1	$6p$
	2	−2, −1, 0, 1, 2	$6d$
	3	−3, −2, −1, 0, 1, 2, 3	$6f$
	4	−4, −3, −2, −1, 0, 1, 2, 3, 4	$6g$
	5	−5, −4, −3, −2, −1, 0, 1, 2, 3, 4, 5	$6h$
$n = 7$	0	0	$7s$
	1	−1, 0, 1	$7p$
	2	−2, −1, 0, 1, 2	$7d$
	3	−3, −2, −1, 0, 1, 2, 3	$7f$
	4	−4, −3, −2, −1, 0, 1, 2, 3, 4	$7g$
	5	−5, −4, −3, −2, −1, 0, 1, 2, 3, 4, 5	$7h$
	6	−6, −5, −4, −3, −2, −1, 0, 1, 2, 3, 4, 5, 6	$7i$

How many electrons could be occupied in the orbitals?
Quantum Number and Electrons!

Name	Symbol	Allowed Values	Property
Principal	n	positive integers 1,2,3…	Orbital size and energy level
Secondary (Angular momentum)	l	Integers from 0 to (n-1)	Orbital shape (sublevels/subshells)
Magnetic	m_l	Integers $-l$ to $+l$	Orbital orientation
Spin	m_s	$+½$ or $–½$	Electron spin Direction

Q: Supply the values of the missing quantum numbers and sublevel names.

	n	l	m_l	*Name*
(i)	?	?	0	4*p*
(ii)	2	1	0	?
(iii)	3	2	-2	?
(iv)	?	?	?	2*s*

Q: According to the concept of the quantum numbers which of the following orbitals are possible and which are not? Give possible explanation against your reasons.

i) 2p ii) 2d iii) 3d iv) 1p

Q: Explain why each of the following sets of quantum numbers is not permissible for an orbital

(i) $n = 0, l = 1, m_l = 0, m_s = +1/2$

(ii) $n = 3, l = 2, m_l = +3, m_s = -1/2$

Q: According to the concept of the quantum numbers which of the following orbitals are possible and which are not? Give possible explanation against your reasons.

i) 2p **ii) 2d** **iii) 3d** **iv) 1p**

Q: Explain why each of the following sets of quantum numbers is not permissible for an orbital

(i) $n = 0, l = 1, m_l = 0, m_s = +1/2$

(ii) $n = 3, l = 2, m_l = +3, m_s = -1/2$

Electronic Configuration of Atoms

In an atom the electrons are held in different orbits, sub-shells and orbital in a regular way. This arrangement of electrons in an atom is called the electronic configuration.

Principles that influence the electronic configuration of atom:

- Pauli's exclusion principle
- Aufbau principle
- Hund's rule

Niels Henrik David Bohr 1885 –1962

Nobel Prize in Physics in 1922

The aufbau method was initially proposed by the Danish physicist **Niels Bohr**, who was the first person to use quantum mechanics to study atomic structure.

Aufbau principle

According to this principle, 'the electrons will **first** occupy the **lowest** energy levels'.

- ❖ The energy of the levels are determined by their (n + l) values.
- ❖ The electron will first occupy the orbital having the lowest value of (n + l)

Q. In which orbital the electron will go first if the values of (n + l) is same for both of the orbital?

Ans: In that case the electron goes to the orbital with lowest value of 'n'.

3d---- n=3, l=2----n+l=5

4s---- n=4,l=0-----n+l=4

3d-----n=3,l=2====5

4p-----n=4,l=1====5

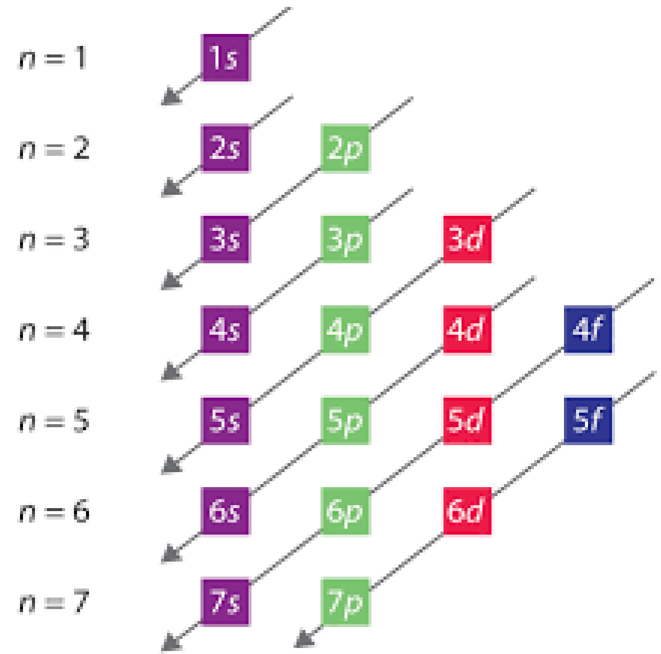


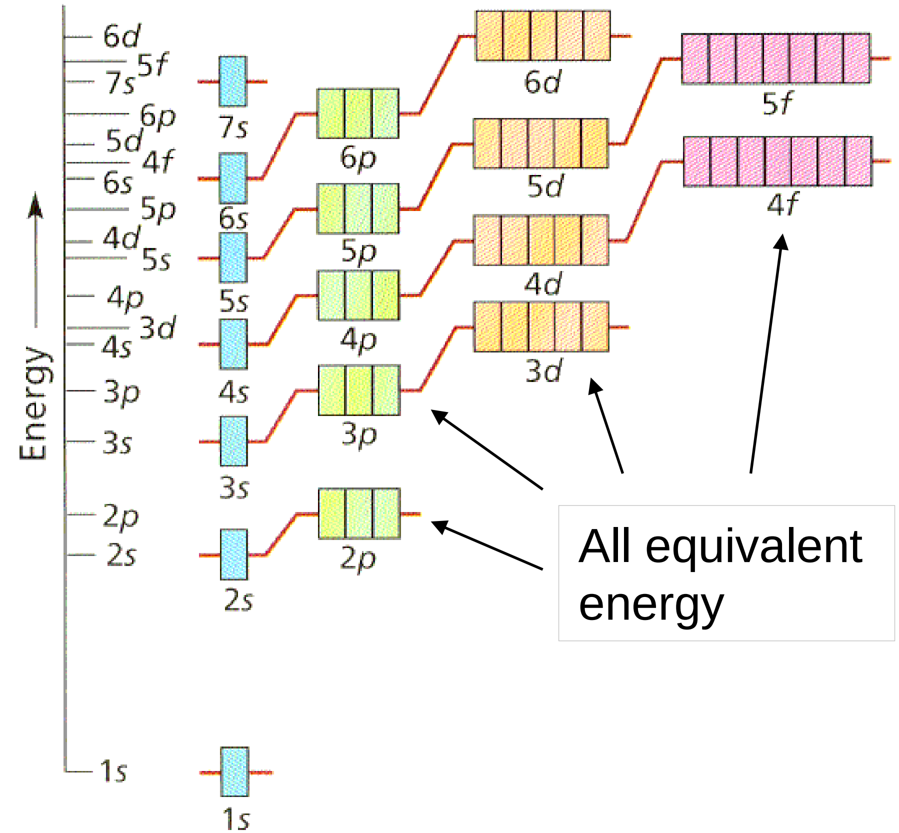
Figure: Filling of electrons in various orbitals according to (n+1) rules

<u>Increasing order of energies of the atomic orbitals:</u>

1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s.............

The Aufbau Principle

Aufbau comes from the German word "aufbauen" meaning "to build." When writing electron configurations, orbitals are built up from atom to atom. When writing the electron configuration for an atom, orbitals are filled in order of increasing atomic number



Each electron occupies the lowest energy orbital

- Electrons are Lazy!!!

All orbitals related to an energy level are of equal energy.

Ex. The three 2p orbitals are the same energy level.

Exceptions to Electron Configurations

A. Copper and chromium are exceptions to the Aufbau principle.

Element	Should be	Actually is
Copper	$1s^2 2s^2 2p^6 3s^2 3p^6 \underline{\mathbf{3d^4 4s^2}}$	$1s^2 2s^2 2p^6 3s^2 3p^6 \underline{\mathbf{3d^5 4s^1}}$
Chromium	$1s^2 2s^2 2p^6 3s^2 3p^6 \underline{\mathbf{3d^9 4s^2}}$	$1s^2 2s^2 2p^6 3s^2 3p^6 \underline{\mathbf{3d^{10} 4s^1}}$

B. Some configurations violate the Aufbau Principle because half-filled sublevels are not as stable as filled sublevels, but they are more stable than other configurations

Unusual Electron Configurations

Element	Predicted Electron Configuration	Actual Electron Configuration
copper, Cu	[Ar] $3d^9\ 4s^2$	[Ar] $3d^{10}\ 4s^1$
silver, Ag	[Kr] $4d^9\ 5s^2$	[Kr] $4d^{10}\ 5s^1$
gold, Au	[Xe] $4f^{14}\ 5d^9\ 6s^2$	[Xe] $4f^{14}\ 5d^{10}\ 6s^1$
palladium, Pd	[Kr] $4d^8\ 5s^2$	[Kr] $4d^{10}$
chromium, C r	[Ar] $3d^4\ 4s^2$	[Ar] $3d^5\ 4s^1$
molybdenum, Mo	[Kr] $4d^4\ 5s^2$	[Kr] $4d^5\ 5s^1$

Wolfgang Pauli 1900-1958

Nobel Prize in Physics 1945

"for the discovery of the Exclusion Principle, also called the Pauli Principle."

Pauli's exclusion principle

According to this principle, 'no two electrons in the same atom can have the same values for the four quantum numbers'.

As an orbital can contain a maximum of only two electrons, the two electrons must have opposing spins. This means if one is assigned an up-spin (+1/2), the other must be down- spin (-1/2).

For example, He (helium) had two electrons in 1s orbital and their electronic configuration is $1s^2$, that means they had two electrons in the 1s orbital. This two electrons can have same values for three of their quantum numbers, but the fourth quantum number must be different for the two electrons.

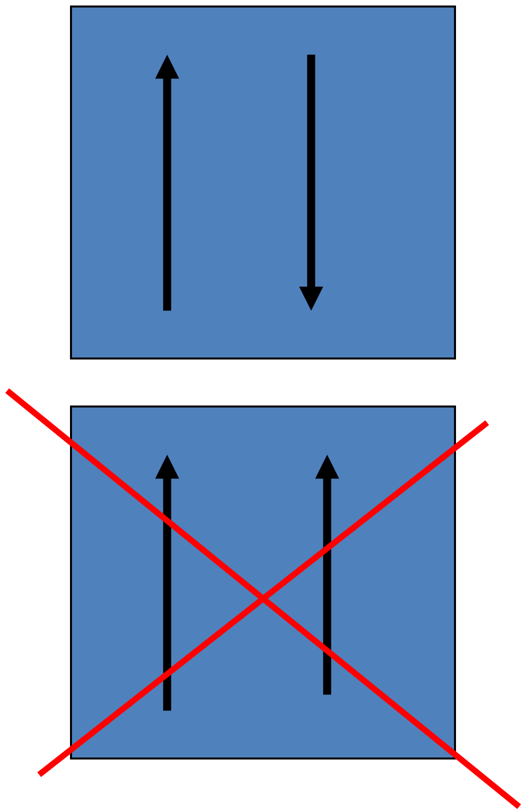
Electronic configuration of helium atom is: He (2) = $1s^2$

For the first electron, $\mathbf{n = 1, l = 0, m_l = 0, m_s = +1/2}$

And for the second electron, $\mathbf{n = 1, l = 0, m_l = 0, m_s = -1/2}$

So, these two electrons have different values of their spin quantum number.

Pauli Exclusion Principle



Box = orbital

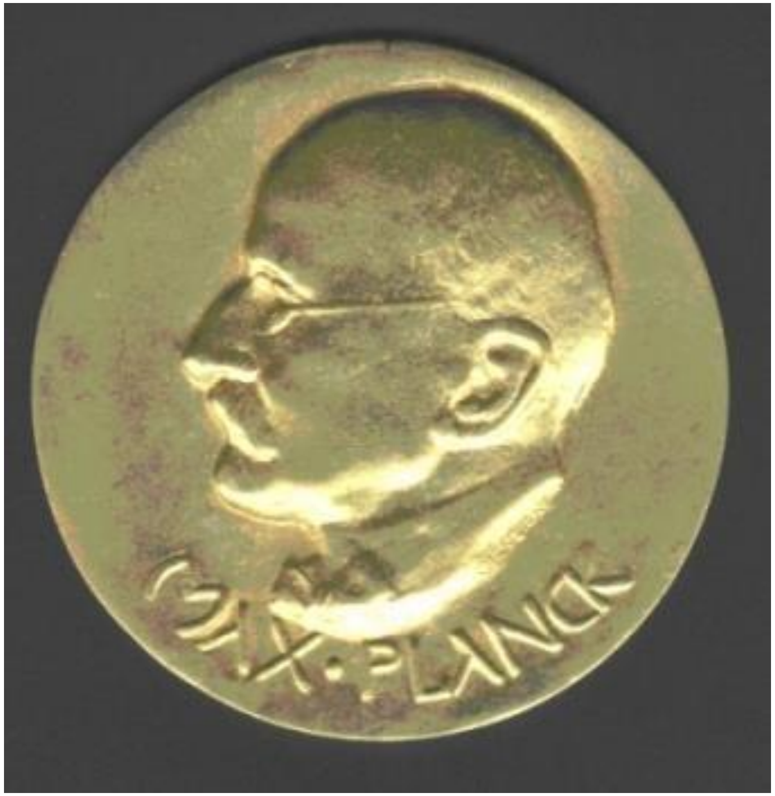
Arrow = electron

A maximum of two electrons may occupy a single orbital, but *only if the electrons have opposite spins.*

- Spin -- Electrons has an associated "spin," either one way or the other, like a top.
- These spins are called "spin up" and "spin down."
- See example on board.

Friedrich Hund 1896-1997

Max Planck Medal in Physics 1943



Hund's rule

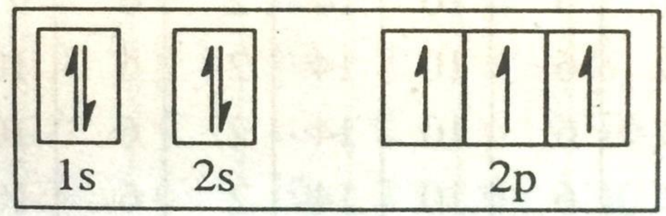
According to this rule, 'electron pairing in any orbital of same sub level will not occur until each orbital contains one electron'.

For example:

Electronic configuration of nitrogen atom is: **N (7) = $1s^2$ $2s^2$ $2p_x^1$ $2p_y^1$ $2p_z^1$**

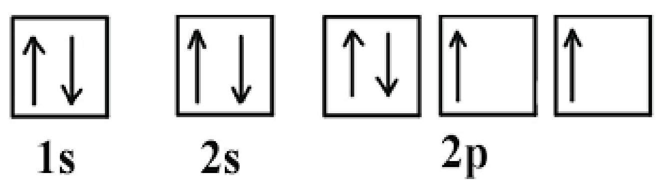
The electrons of p orbital will be equally distributed in three p orbital ant the configuration of N will be:

$1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$. In writing using box system it will be as follows:



In case of O_2 the electron distribution will be:

O (8) = $1s^2$ $2s^2$ $2p_x^2$ $2p_y^1$ $2p_z^1$



The fourth electron become paired up in p_x and is of opposite spin as electron of same spin repel each other.

Hund's rule states that:

1. Every orbital in a sublevel is singly occupied before any orbital is doubly occupied.
2. All of the electrons in singly occupied orbitals have the same spin (to maximize total spin).

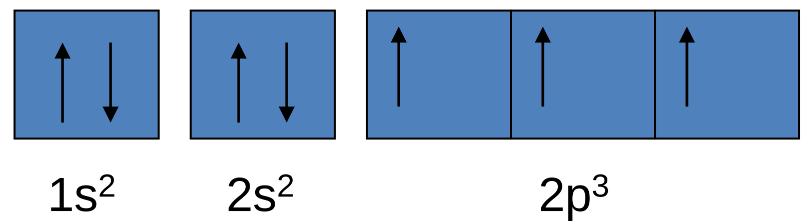
Single electrons with the *same* spin must occupy each equal-energy orbital *before* additional electrons with opposite spins can occupy the *same* orbitals.

- Electrons are **UNFRIENDLY**.

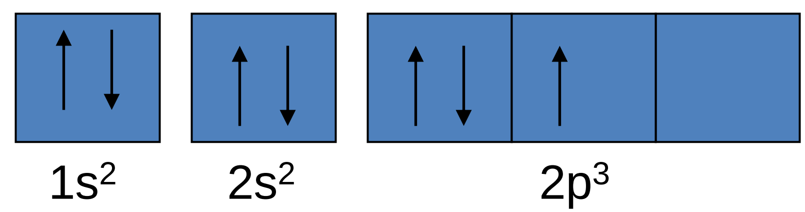
Why?

Ex. Nitrogen:

• $1s^2\ 2s^2\ 2p^3$



NOT



Electronic configuration of elements following Hund’s rule

Elements	Atomic	Electronic configuration	Box System
H	1	$1s^1$	1s [↑]
He	2	$1s^2$	1s [↑↓]
Li	3	$1s^2\ 2s^1$	1s [↑↓] 2s [↑]
Be	4	$1s^2\ 2s^2$	1s [↑↓] 2s [↑↓]
B	5	$1s^2\ 2s^2\ 2p^1$	1s [↑↓] 2s [↑↓] 2p [↑][ ][ ]
C	6	$1s^2\ 2s^2\ 2p^2$	1s [↑↓] 2s [↑↓] 2p [↑][↑][ ]
N	7	$1s^2\ 2s^2\ 2p^3$	1s [↑↓] 2s [↑↓] 2p [↑][↑][↑]
O	8	$1s^2\ 2s^2\ 2p^4$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑][↑]
F	9	$1s^2\ 2s^2\ 2p^5$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑]
Ne	10	$1s^2\ 2s^2\ 2p^6$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓]
Na	11	$1s^2\ 2s^2\ 2p^6\ 3s^1$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓] 3s [↑]
Mg	12	$1s^2\ 2s^2\ 2p^6\ 3s^2$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓] 3s [↑↓]
Al	13	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓] 3s [↑↓] 3p [↑][ ][ ]
Si	14	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓] 3s [↑↓] 3p [↑][↑][ ]
P	15	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓] 3s [↑↓] 3p [↑][↑][↑]
S	16	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓] 3s [↑↓] 3p [↑↓][↑][↑]
Cl	17	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓] 3s [↑↓] 3p [↑↓][↑↓][↑]
Ar	18	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$	1s [↑↓] 2s [↑↓] 2p [↑↓][↑↓][↑↓] 3s [↑↓] 3p [↑↓][↑↓][↑↓]

Shell	Principal quantum number (n)	maximum number of electron in a shell (orbital) $2n^2$	Azimuthal quantum number (l) = 0,1.... (n-1)	Maximum no. of electron in a orbital $2(2l+1)$	Magnetic quantum number (m) different possible orientation of orbital	Designation of orbitals in a given shell
K	1	$2(1)^2 = 2$	0	$2[2(0)+1] = 2$	0	1s
L	2	$2(2)^2 = 8$	0	2	0	2s
			1	$2[2(1)+1] = 6$	-1, 0, +1	$2p_y$, $2p_z$, $2p_x$
M	3	$2(3)^2 = 18$	0	2	0	3s
			1	6	-1, 0, +1	$3p_y$, $3p_z$, $3p_x$,
			2	$2[2(2)+1] = 10$	-2, -1, 0, +1, +2	$3d_{x^2-y^2}$, $3d_{yz}$, $3d_{z^2}$, $3d_{zx}$, $3d_{xy}$
N	4	$2(4)^2 = 32$	0	2	0	4s
			1	6	-1, 0, +1	$4p_y$, $4p_z$, $4p_x$
			2	10	-2, -1, 0, +1, +2	$4d_{x^2-y^2}$, $4d_{xy}$, $4d_{z^2}$, $4d_{yz}$, $4d_{zx}$
			3	$2[2(3)+1] = 14$	-3, -2, -1, 0, +1, +2, +3	$f_{y(3x^2-y^2)}$, $f_{z(x^2-y^2)}$, f_{yz^2}, f_{z^3}, f_{xz^2}, f_{xyz}, $f_{x(x^2-3y^2)}$

The labels on the orbitals, such as p_x, d_{z^2}, f_{xyz} etc. are not associated with specific 'm' values

Thanks to All