



Ministry of Higher Education and Scientific Research

Al-Muthanna University

Inorganic Pharmaceutical chemistry

For the 3rd year students of the «faculty of Pharmacy»

Lecture (1)

Atomic structure part 1

Dr. Rusul Alabada



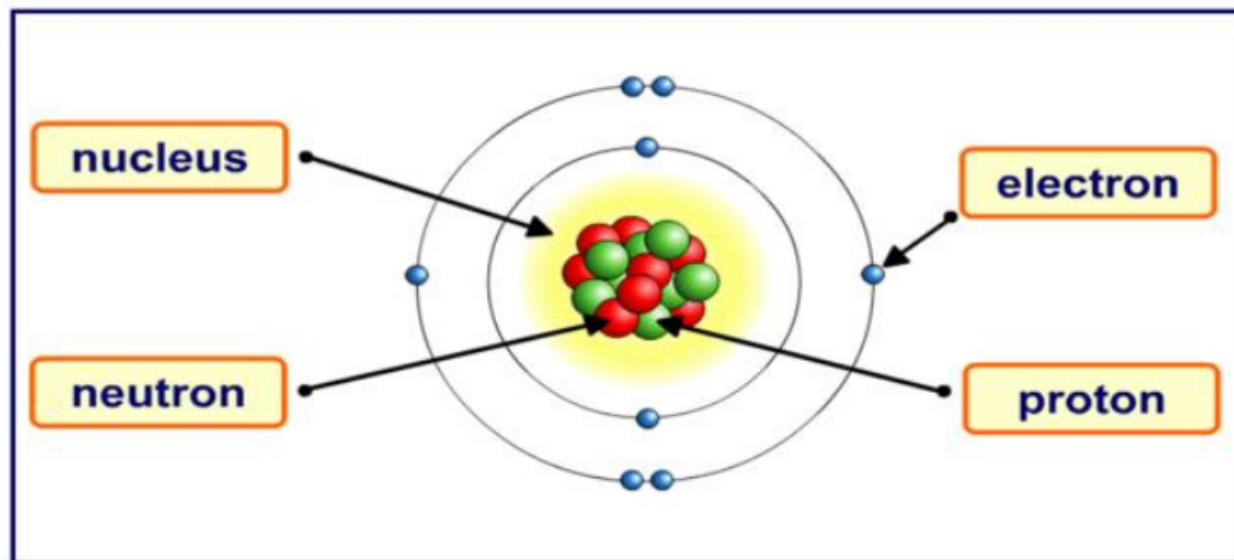
Electronic Structure of Atoms

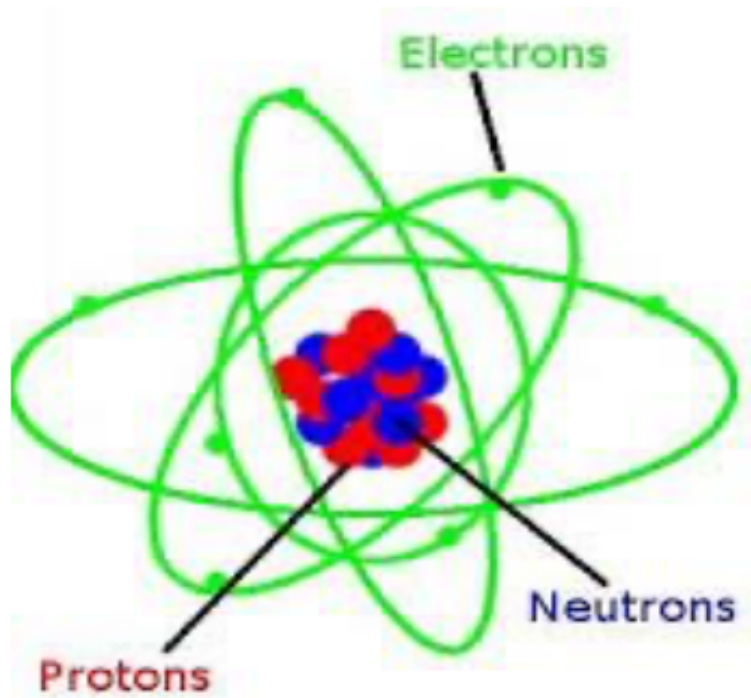
The fundamental unit of all matter is the atom. The various chemical and physical properties of matter are determined by its elemental composition. Elements are composed of like atoms and their isotopes.

To predict the properties of matter, molecules, or elements, it is important to understand the structure of atoms.

Subatomic Particles

- ▶ Atom is composed of a **nucleus** at the center which contains most of the mass of the atom, and orbiting **electrons** (negatively charged particles), which have negligible mass.
- ▶ The nucleus is composed of **protons** (positively charged particles), and **neutrons** (uncharged particles).
- ▶ The radius of the diameter





$$\begin{array}{c}
 \text{Number of} \\
 \text{Neutrons}
 \end{array}
 +
 \begin{array}{c}
 \text{Number of} \\
 \text{Protons}
 \end{array}
 =
 \begin{array}{c}
 \text{Mass} \\
 \text{Number}
 \end{array}$$

Particles	Mass	Relative mass	Charge
Proton	1.675×10^{-24} g	1	+1
Neutron	1.675×10^{-24}	1	0
Electron	9.107×10^{-28}	1/1836	-1

► Atoms can be described by two numbers:

1. The atomic number (Z), which is equal to the number of protons the atom contains.

Ex: Hydrogen's atomic number is 1, So hydrogen has 1 proton

Ex: Carbon's atomic number is 6, So carbon has 6 protons

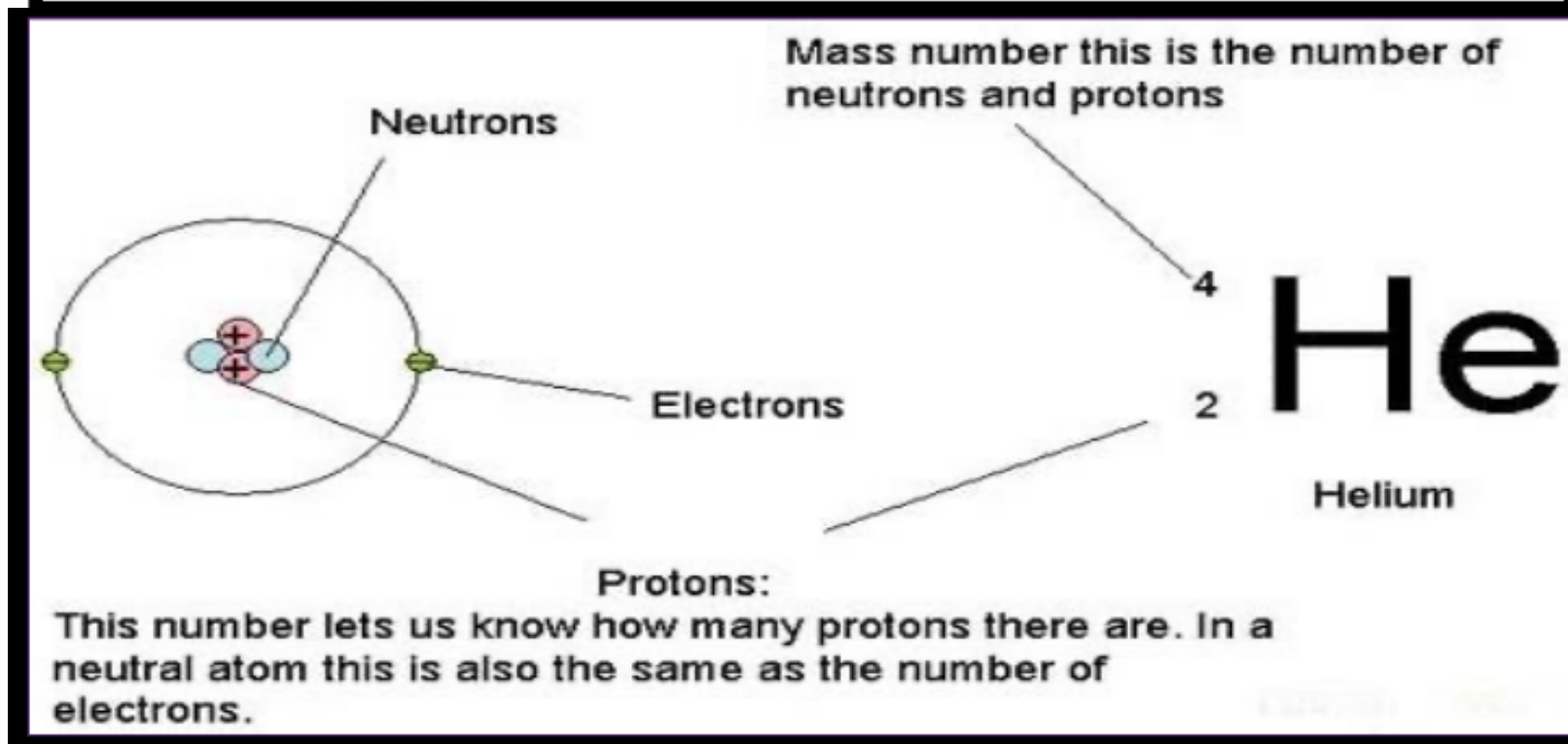
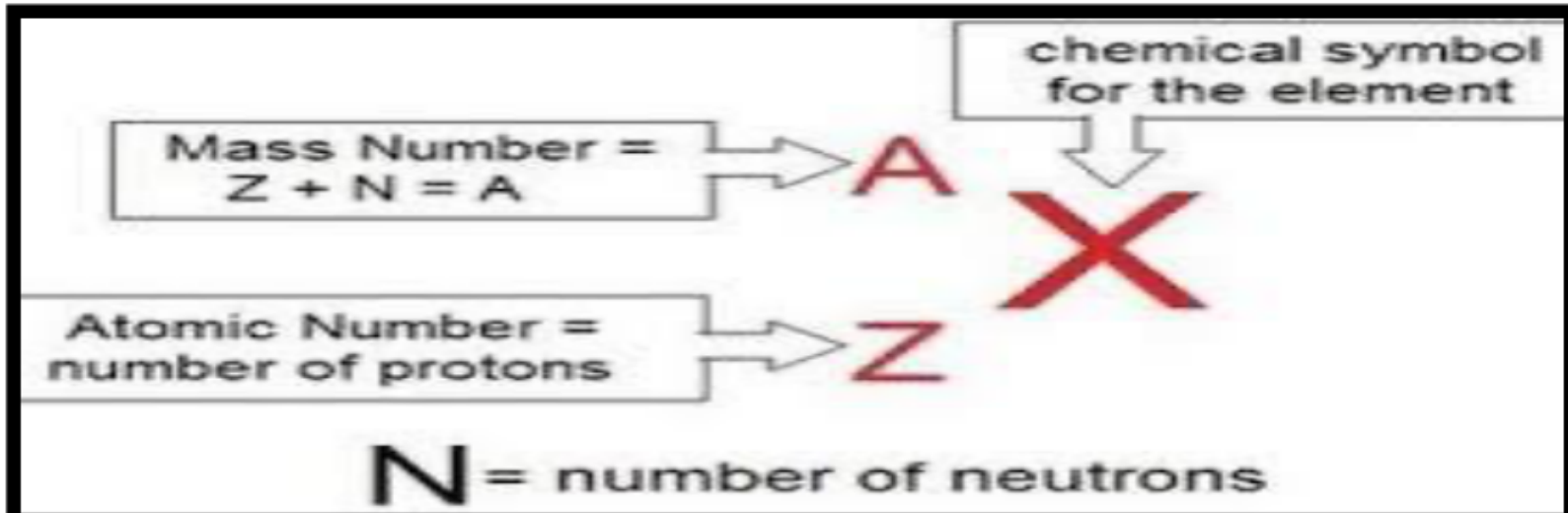
*The number of protons identifies the atom.

Ex. 2 protons = He, 29 protons = Cu

No. of protons = ATOMIC NUMBER of the atom (proton number)

2. The mass number (A), which is equal to the number of protons plus neutrons

No. of protons + no of neutrons = MASS NUMBER

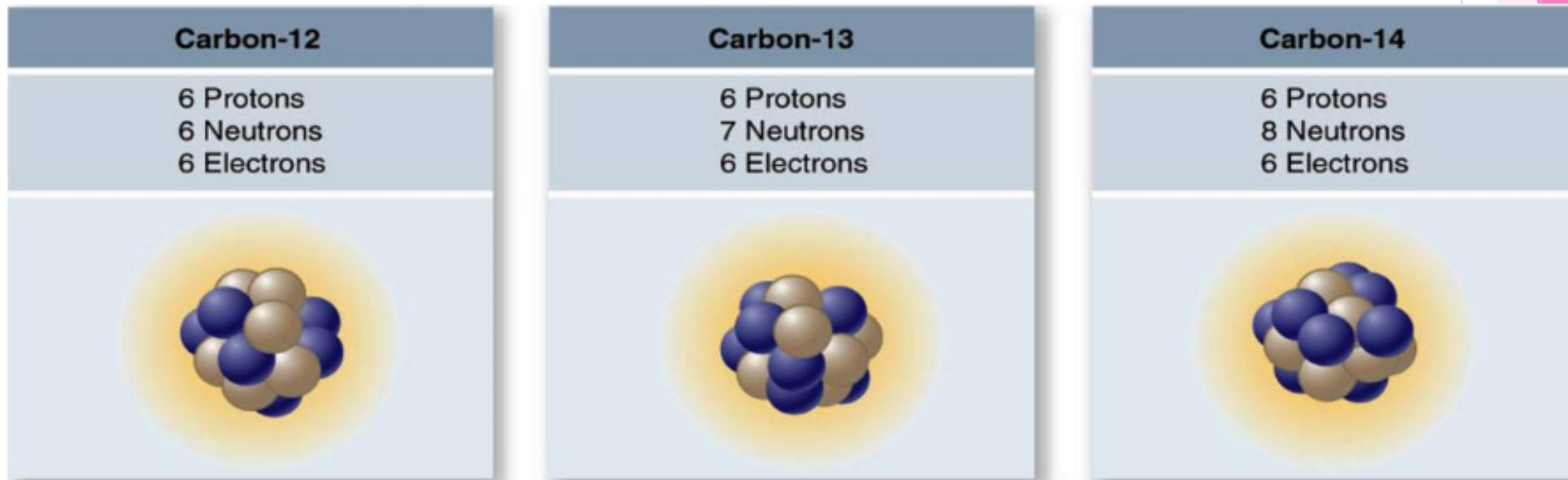


- ▶ Example: $^{19}_9\text{F}$ The atomic number counts the number of protons (9); the mass number counts protons + neutrons (19). If there are 9 protons, there must be 10 neutrons for the total to add up to 19.
- ▶ K has a mass number of 39 and an atomic number of 19

$$P = 19 \quad n = 20 \quad e = 19$$

Isotopes

The number of neutrons in an atom can vary within small limits. For example, there are three kinds of carbon atom ^{12}C , ^{13}C and ^{14}C . They all have the same number of protons, but the number of neutrons varies. Isotopes are atoms which have the same atomic number but different mass numbers.



Atomic Orbitals

- ▶ **Heisenberg Principle** - states that it is impossible to define what time and where an electron is and where is it going next. This makes it impossible to know exactly where an electron is traveling in an atom.

Since it is impossible to know where an electron is at a certain time, a series of

calculations are used to approximate the volume and time in which the electron can

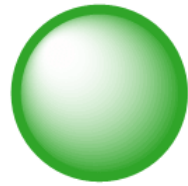
be located. These regions are called Atomic Orbitals. These are also known as the

quantum states of the electrons.

- Only two electrons can occupy one orbital and they must have different spin states, $\frac{1}{2}$ spin and $-\frac{1}{2}$ spin (easily visualized as opposite spin states).

Atomic Subshells

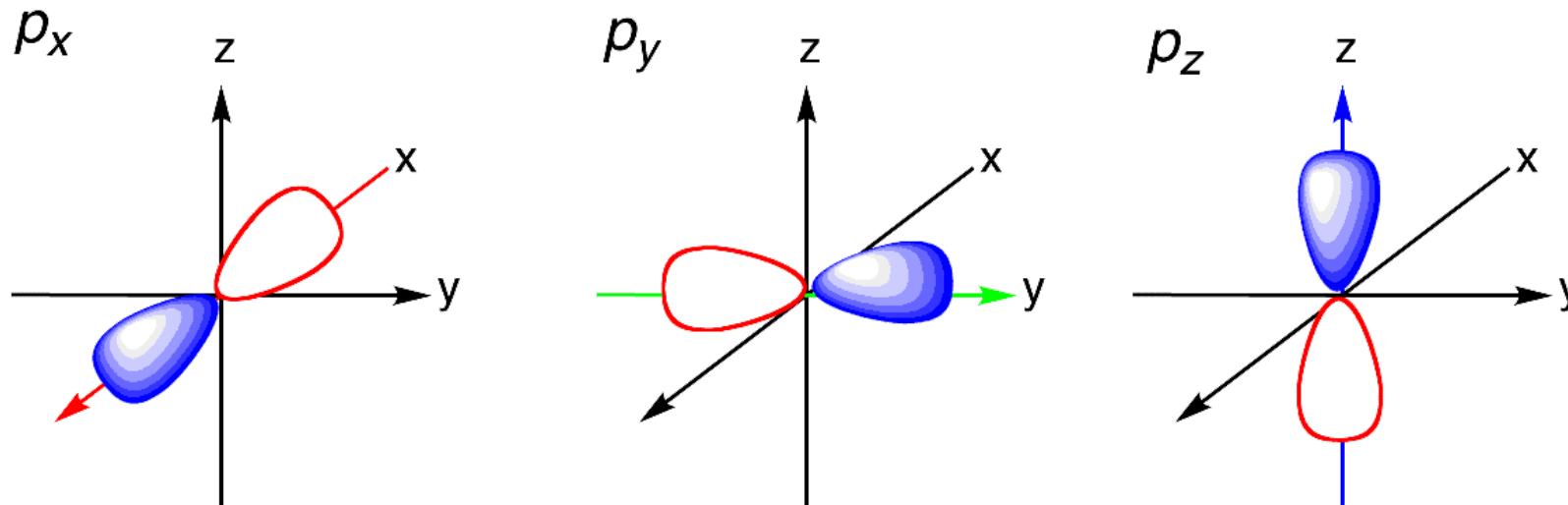
- ▶ These are some examples of atomic orbitals:
- ▶ **S subshell:** (Spherical shape) There is one S orbital in an S subshell. The electrons can be located anywhere within the sphere centered at the atom's nucleus.



S

P Orbitals

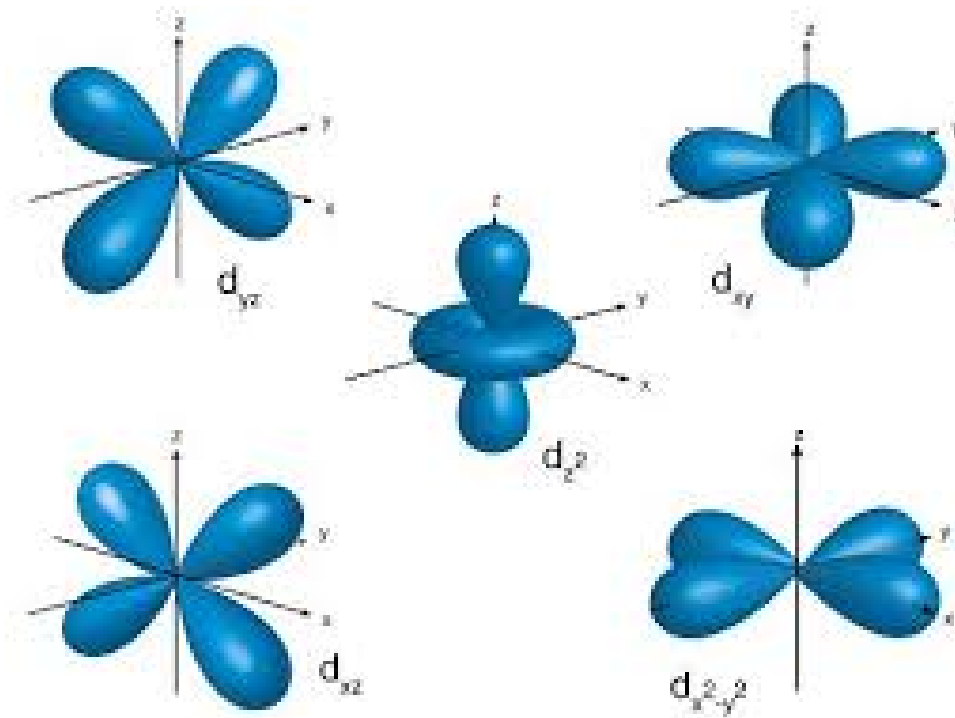
- ▶ **P Orbitals:** (Shaped like two balloons tied together) There are 3 orbitals in a p subshell that are denoted as p_x , p_y , and p_z orbitals. These are higher in energy than the corresponding S orbitals.



The three p orbitals are aligned along perpendicular axes

D Orbitals

- ▶ **D Orbitals:** The d subshell is divided into 5 orbitals (d_{xy} , d_{xz} , d_{yz} , d_{z^2} and $d_{x^2-y^2}$). These orbitals have a very complex shape and are higher in energy than the S and P orbitals.



Rules for determining the structure of any particular atoms:

▶ **Aufbau process**

Means to build up. When writing electron configurations, we are building up electron orbitals.

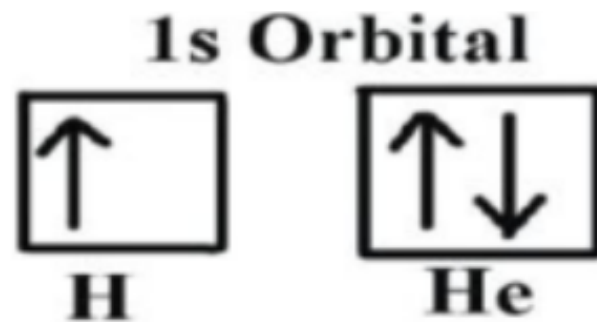
Before the process can be properly employed, there are some fundamental rules that must be followed.

□ **Pauli Exclusion Principle**

States that in any atom, no two electrons can have the same four quantum numbers. (this means that no more than two electrons can occupy the same orbital, and that two electrons in the same orbital must have opposite spins)

► Example

We have the first three quantum numbers $n=1$, $l=0$, $m_l=0$. Only two electrons can correspond to these, which would be either $m_s = -1/2$ or $m_s = +1/2$. We can conclude that these four quantum numbers refer to 1s subshell. If only one of the m_s values are given then we would have 1s¹ (denoting Hydrogen) if both are given we would have 1s² (denoting Helium).



Hund's Rule

1- Lower energy orbitals must be filled before higher energy orbitals.

2- Each electron will first fill all the degenerated orbitals (orbitals with similar energy) before pairing with another electron in a half-filled orbital.



Best Regards!

Thank you!