

MOHAMED KHIDER UNIVERSITY OF BISKRA.
FACULTY OF EXACT SCIENCES AND NATURAL AND LIFE SCIENCES
DEPARTMENT OF BIOLOGY

COURSE TITLE: General Chemistry I
CHAPTER III: Part 1 and 2
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Dr: Ismail DAOUD

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1.3. Electronic configuration of atoms

1.3.1. Introduction to quantum numbers

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1.3. Electronic configuration of atoms

1.3.1. Introduction to quantum numbers

The modern theory of the electronic structure of the atom stems from a complex mathematical equation (called the Schrodinger equation), which is beyond the mathematical requirements for the general chemistry course. The solution of this equation yields three *quantum numbers*, with a fourth and final quantum number obtained from experimental results.

Each electron is specified in terms of its four quantum numbers that govern its energy, its orientation in space, and its possible interactions with other electrons.

The four quantum numbers values describe the probable location of the electron.

Finally, to write the electronic structure expression of an atom, it is necessary to learn:

- (1) The names, symbols, and permitted values of the quantum numbers.
- (2) The order of increasing energy of electrons as a function of their sets of quantum numbers.

The four quantum numbers are named and have describe as revealed in Table 1

Table 1 : Quantum Numbers

Name	Symbol	Limitations	Definitions
Principal quantum number	n	$n \geq 1$ ($n=1, \dots, 7$)	-Shell: ($n=1$ k, $n=2$, l, $n=3$, M, ..., $n=7$, Q). -Line (period) of periodic table. -Determinate the energy of the electron ($E_n = -13.6/n^2 \Rightarrow$ Energy level). - Electron numbers ($2n^2$) -Orbital atomic numbers (n^2)
Angular momentum quantum number or Azimuthal quantum number	l	$0 \leq l \leq n - 1$	-Subshell: ($l=0$, S, $l=1$, P, $l=2$, d, $l=3$, f). -Shape of Orbital. - $l=0 \Rightarrow S \Rightarrow$ Sphere - $l=1 \Rightarrow P \Rightarrow$ Lobe - $l=2 \Rightarrow d \Rightarrow$ Deux lobes - $l=3 \Rightarrow f \Rightarrow$ Trois lobes
Magnetic quantum number	m_l	$-l \leq m_l \leq +l$	- Determines the orientation in space of the

			electron - Orbital atomic numbers (n^2) \Rightarrow (Cases). - $l=0 \Rightarrow S \Rightarrow -0 \leq m_l \leq +0 \Rightarrow \square$ - $l=1 \Rightarrow P \Rightarrow -1 \leq m_l \leq +1 \Rightarrow \square\square\square$ - $l=2 \Rightarrow d \Rightarrow -2 \leq m_l \leq +2 \Rightarrow \square\square\square\square\square$ - $l=3 \Rightarrow f \Rightarrow -3 \leq m_l \leq +3 \Rightarrow \square\square\square\square\square\square\square$
Spin quantum number	m_s	$+1/2, -1/2$	- Determines the orientation of the electron in axis within the case. - $m_s = +1/2 \Rightarrow \boxed{\uparrow}$, $m_s = -1/2 \Rightarrow \boxed{\downarrow}$

Example:

Determine the other quantum numbers associated with the principal quantum number value $n=3$.

Solution:

$n=3 \Rightarrow$ Shell : M

$$0 \leq l \leq n - 1$$

$\Rightarrow 0 \leq l \leq 2 \Rightarrow l=0$ (Subshell : s), $l=1$ (Subshell : p), $l=2$ (Subshell : d)

$$-l \leq m_l \leq +l$$

$$l=0 \Rightarrow -0 \leq m_l \leq +0 \Rightarrow \square$$

$$l=1 \Rightarrow -1 \leq m_l \leq +1 \Rightarrow \square\square\square$$

$$l=2 \Rightarrow -2 \leq m_l \leq +2 \Rightarrow \square\square\square\square\square$$

1.3.2. Principles governing the electronic structure of an atom:

The n and l quantum numbers determine the energy of each electron. The energies of the electrons increase as the sum $n+l$ increases; the lower the value of $n+l$ for an electron in an atom, the lower is its energy.

The order of increasing energy is as follows:

1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d.

$1s(n=1, l=0) \Rightarrow (n+l=1)$, $2p(n=2, l=1) \Rightarrow (n+l=3)$.

1s,	2s,	2p,	3s,	3p,	4s,	4p
($n+l=1$)	($n+l=2$)	($n+l=3$)	($n+l=3$)	($n+l=4$)	($n+l=4$)	($n+l=5$)
$n=1$	$n=2$	$n=2$	$n=3$	$n=3$	$n=4$	$n=4$

Example: For two electrons with equal values of $n+l$, the one with the lower n value has lower energy. Thus, we can fill an atom with electrons starting with its lowest-energy electrons by starting with the electrons with the lowest sum $n+l$.

a. Energy rule (Klechkowski rule)

Thus, an important development has occurred because of the $n+l$ rule.

The energies of the various subshells are plotted along the vertical axis. The subshells are displaced left to right merely to avoid overcrowding. The order of increasing energy is as follows:

$1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d$.

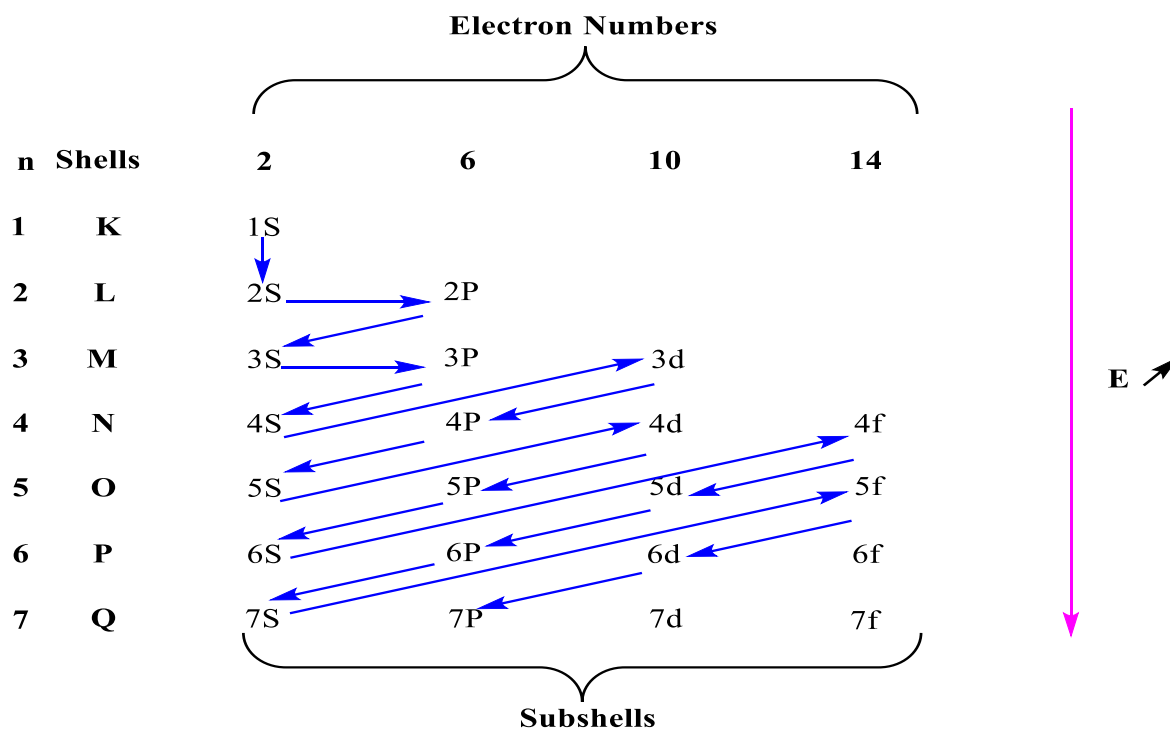


Figure 1 : Order of allocation of subshells to electrons according to Klechkowski rule

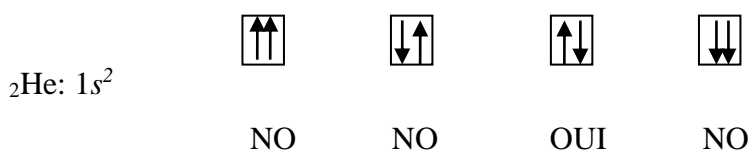
Note: Experience has shown that this rule has certain exceptions.

b. Pauli exclusion rule

“An atomic orbital (OA=Case) can only contain a maximum of 2 electrons in this case will have opposite spins”

The *Pauli exclusion principle* states that no two electrons in the same atom can have the same set of four quantum numbers. Along with the order of increasing energy, we can use this principle to deduce the order of filling of electron shells in atoms.

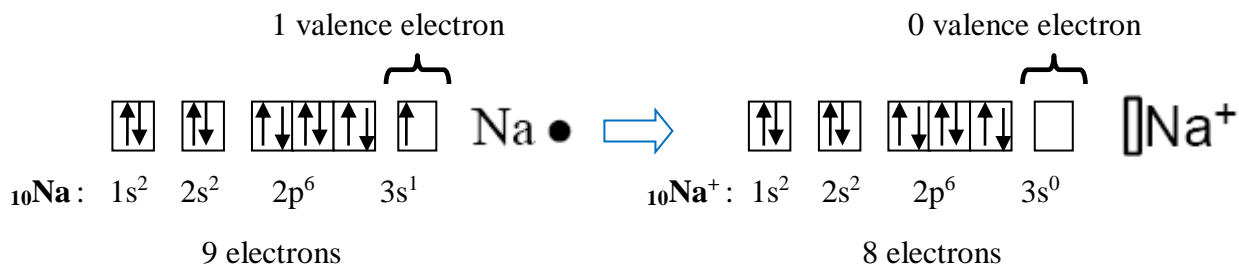
Example:





Elimination of one or more electrons from the electronic configuration of the atom in its ground state while respecting the rules of Klechkowski, Pauli and Hund.

Exemple : Sodium ion: ${}_{11}\text{Na}^+$



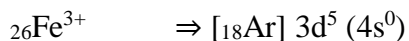
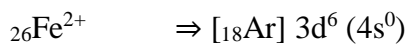
Consequence of subshell inversions:

Exemples : Iron ions : ${}_{26}\text{Fe}^{2+}$ et ${}_{26}\text{Fe}^{3+}$

(Reversal done)



Consequence: The 4s subshell “empties” before the 3d subshell.



Identical reasoning for compounds with electrons in their 4d, 4f or 5f subshells. We first empty the 5s, 6s or 7s subshells.