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General Chemistry

CHAPTER II: ELECTRONIC CONFIGURATION OF ATOMS

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1.3. Electronic configuration of atoms

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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	$n \geq 1 \quad (n=1,\ldots\ldots 7)$	-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 ⇒ 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 ⇒ S ⇒ Sphere - l=1 ⇒ P ⇒ Lobe - l=2 ⇒ d ⇒ Deux lobes - l=3 ⇒ f ⇒ 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) ⇒ (Cases). - l=0 ⇒ S ⇒$-0 \leq m_l \leq +0$ ⇒ □ - l=1 ⇒ P ⇒$-1 \leq m_l \leq +1$⇒ □□□ - l=2 ⇒ d ⇒$-2 \leq m_l \leq +2$⇒ □□□□□ -l=3 ⇒ f ⇒$-3 \leq m_l \leq +3$⇒ □□□□□□□
Spin quantum number	m_s	+½, -½	- Determines the orientation of the electron in axis within the case. - m_s=+½ ⇒ ↑, - m_s=-½ ⇒ ↓

Example:

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

Solution:

n=3 ⇒ Shell : M

$0 \leq l \leq n-1$

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

$-l \leq m_l \leq +l$

l= 0 ⇒ $-0 \leq m_l \leq +0$ ⇒ □

l=1 ⇒ $-1 \leq m_l \leq +1$ ⇒ □□□

l=2 ⇒ $-2 \leq m_l \leq +2$ ⇒ □□□□□

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:

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

1*s*(*n=1, l=0*) ⇒ (*n+l=1*), 2*p*(*n=2, l=1*) ⇒ (*n+l=3*).

1*s*,	2*s*,	2*p*,	3*s*,	3*p*,	4*s*,	4*p*
(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:

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

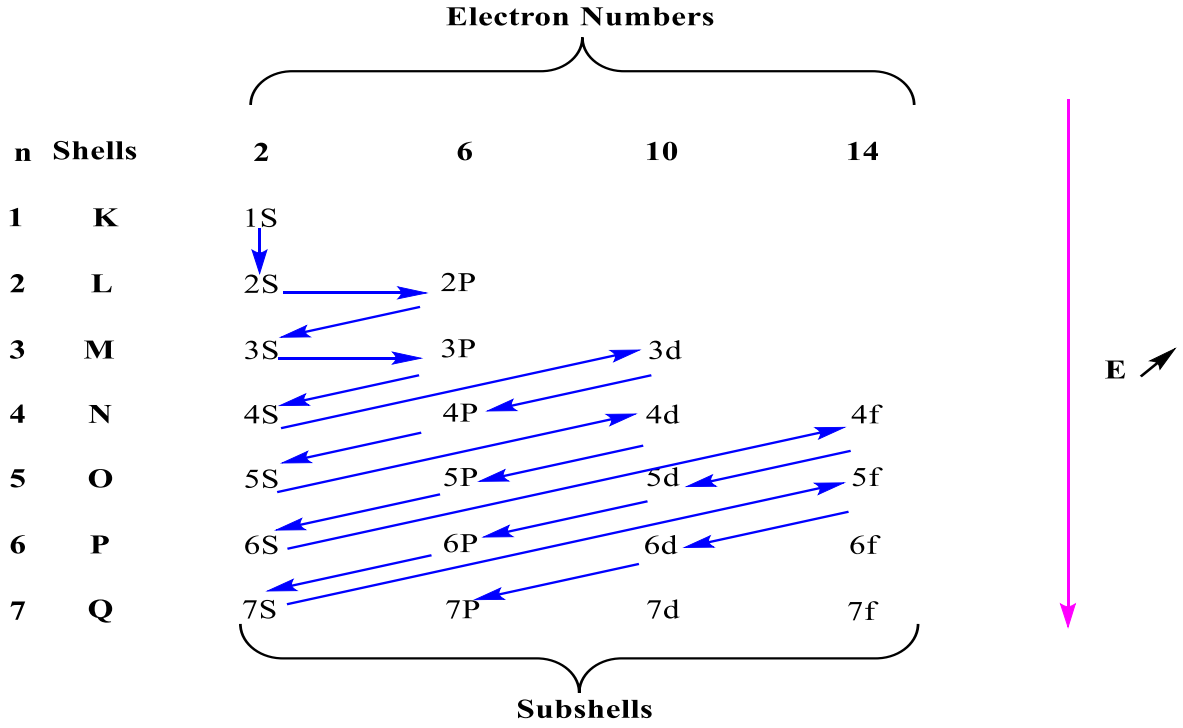


Figure 1 : Order of allocation of subshells to electrons according to Klechkowski rule

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:

$_2$He: $1s^2$



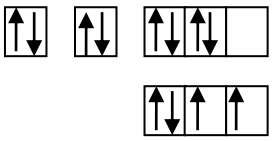
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c. Hund's Rule: (*rule of maximum multiplicity*)

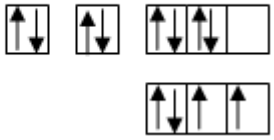
In the same subshell (*p*, *d*, or *f*) the electrons tend to fill the maximum of the quantum boxes with parallel spins (the electrons stay unpaired as much as possible).

Thus the configuration of the oxygen is as follows:

Example: $_8$O: $1s^2$, $2s^2$, $2p^4$



Example: $_8$O: $1s^2$, $2s^2$, $2p^4$



1.3.3. Electronic configuration (Electronic structure):

Writing atomic orbitals with, as a superscript, the number of electrons they contain is called electronic structure. It is based on the Klechkowski diagram.

$_2$He: $1s^2$

$_8$O: $1s^2/\ 2s^2\ 2p^4$

$_{26}$Fe: $1s^2/\ 2s^2 2p^6/3s^2 3p^6/4s^2\ 3d^6$

1.3.4. Limitations of Klechkowski Rule and Exceptions to Filing Rules

a. Subshells inversions

Among the exceptions to the Klechkowski rule is the inversion of the 4s and 3d subshells, i.e. a variation of the order of Klechkowski rule.

Please note: the 4s subshell does have its 2 electrons even if the 3d subshell is not complete.

$_{26}$Fe: $1s^2/\ 2s^2 2p^6/3s^2 3p^6/4s^2\ 3d^6$ $\Rightarrow$ inversion of the 4s and 3d $\Rightarrow$ $_{26}$Fe: $1s^2/\ 2s^2 2p^6/3s^2 3p^6/\ 3d^6\ 4s^2$

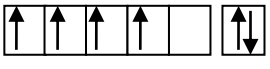
Note: The inversion is identical for subshells: 5s and 4d (then 6s and 4f, then 7s and 5f, etc.).

b. Exceptions to Klechkowski Filling Rules

The subshell d is more stable when it is full (d^{10}) or half full (d^5), a rule valid only for this subshell (case of the chromium and copper groups).

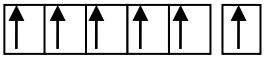
Case of chromium ($_{24}$Cr):

$_{24}$***Cr :*** $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^4\ 4s^2$ $\Rightarrow$ $_{24}$***Cr :*** $[_{18}Ar]\ 3d^4\ 4s^2$



Experimentally

$\Rightarrow$ $_{24}$***Cr :*** $[_{18}Ar]\ 3d^5\ 4s^1$



Case of copper ($_{29}$Cu):

$_{29}$***Cu :*** $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^9\ 4s^2$ ⇒ $_{29}$***Cu :*** $[_{18}Ar]\ 3d^9\ 4s^2$

Experimentally

⇒ $_{29}$***Cu :*** $[_{18}Ar]\ 3d^{10}\ 4s^1$

1.3.5. Core and valence electrons Lewis representation of an atom

Valence electrons are the electrons of the external shell (peripheral or valence).

$_6$C: $1s^2\ /2s^2\ 2p^2$

Valence number is: 4

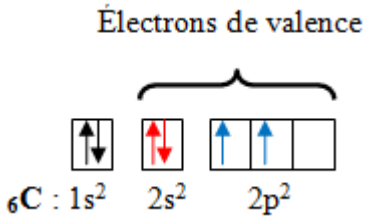
Valence electrons are : 4 e-

Core electrons: 2

The Lewis representation of atoms only takes into account valence electrons. Single electrons are represented by dots and electron doublets are represented by dashes.

According to the Lewis representation, an empty valence OA can be represented by an empty rectangle (= electronic vacancy).

$_6$C: $1s^2\ /2s^2\ 2p^2$

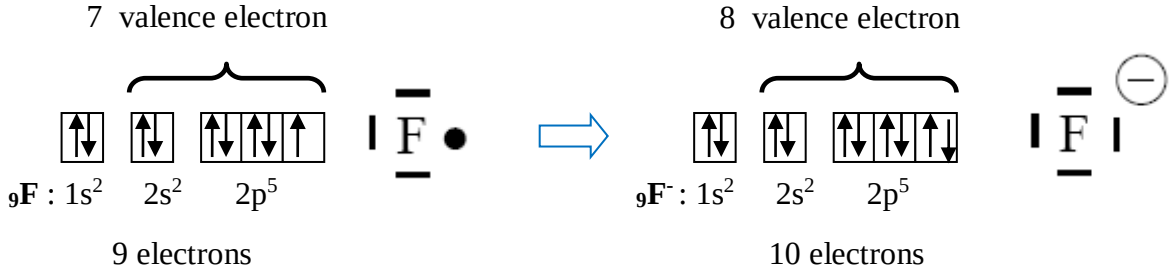


1.3.6. Electronic configuration of an ion

a. Case of anions

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

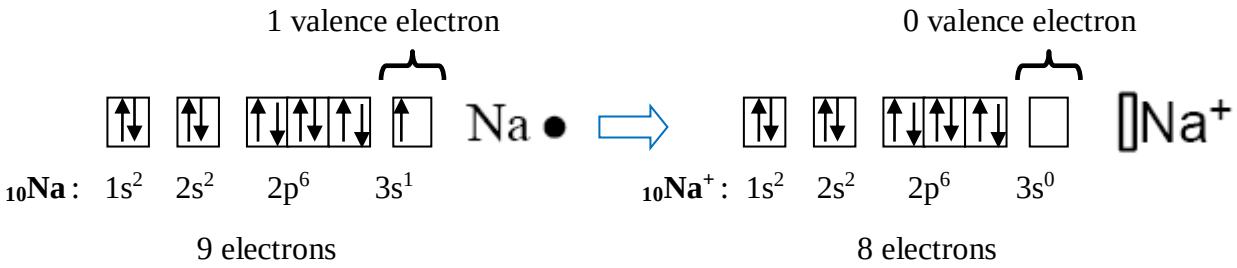
Exemple : Fluoride ion: $_9F^-$



b. Case of cations

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: $_{11}Na^{+}$



Consequence of subshell inversions:

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

(Reversal done)

$_{26}Fe$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \mathbf{3d^6 4s^2}$ ⇒ $[_{18}Ar]\ 3d^6\ 4s^2$

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

$_{26}Fe^{2+}$ ⇒ $[_{18}Ar]\ 3d^6\ (4s^0)$
$_{26}Fe^{3+}$ ⇒ $[_{18}Ar]\ 3d^5\ (4s^0)$

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