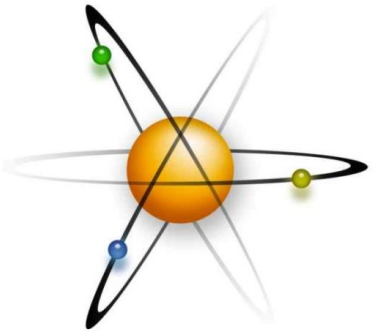
THE CONCEPT OF BIOGENICITY OF CHEMICAL ELEMENTS



Lecture №8

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Krasnoyarsk 2020

WHAT WILL WE STUDY?

- Basic concepts of the topic
- Electronic configurations of atoms of biogenic elements
- Covalent bonds of σ- and π-type and molecular structure

RELEVANCE

- Chemical elements that are necessary for the construction and life of cells and organisms are called **biogenic elements**. All living systems are based on six elements: carbon **C**, hydrogen **H**, oxygen **O**, nitrogen **N**, phosphorus **P**, and sulfur **S**, which are called **organogens** (97% of them).

- In addition, vital **macroelements** also include s-elements of the third (sodium, magnesium) and fourth (potassium, calcium) periods, and p-elements of the third period (chlorine).

AIM

- The aim is to show an **approach** to the study of the properties of chemical elements, based on the electronic structure of atoms and their position in the periodic table, **which is necessary for the subsequent study of complex metabolic processes in the body**

THE STRUCTURE OF THE ATOM AND THE ELECTRON SHELL OF THE ATOM

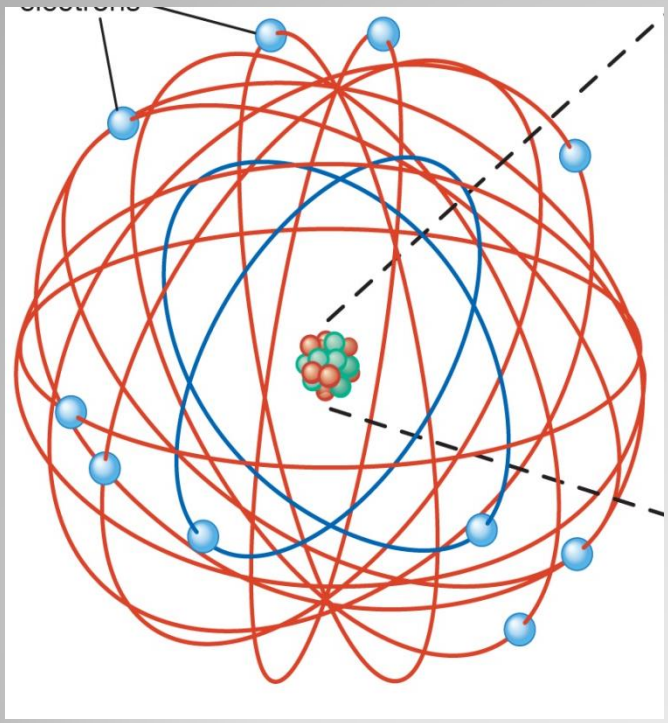
1. The concept of "atom" came to us from ancient times, but completely changed the original meaning that the **ancient Greeks** put into it (in translation from ancient Greek, "atom" means "indivisible"),
2. **Dmitry Ivanovich Mendeleev** (1869, Periodic law of D. I. Mendeleev),
3. **Wilhelm Roentgen** (1895, Discovery of x-rays)

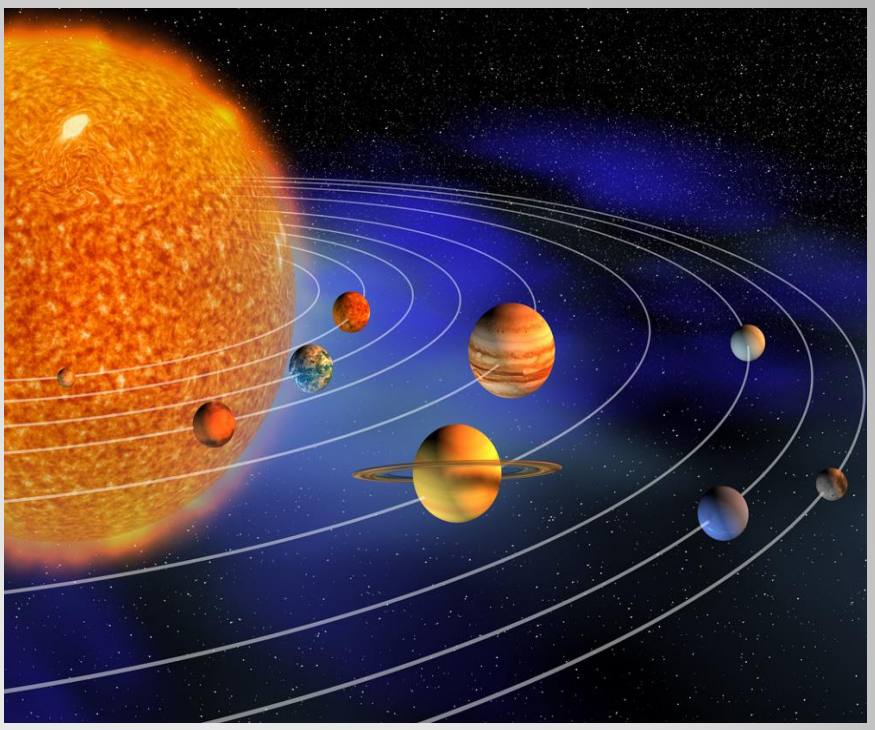
THE STRUCTURE OF THE ATOM AND THE ELECTRON SHELL OF THE ATOM

4. **John Thomson** (1897, discovery of the electron),
5. **Henri Becquerel, Pierre and Marie Curie** (1896-1898, Discovery of radioactivity)…

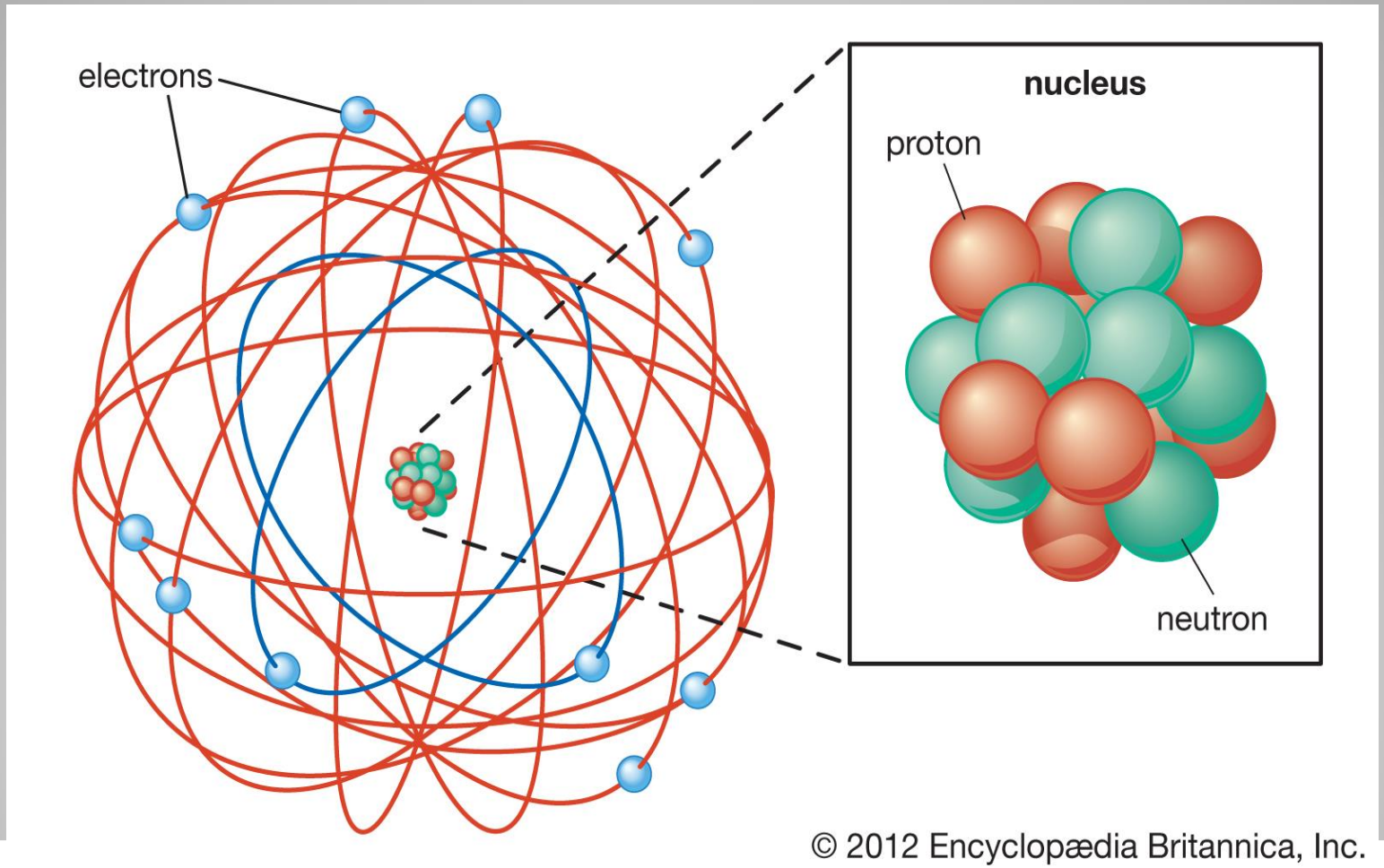
atom is not an indivisible particle, but has a complex structure

- **Ernest Rutherford's** creation of the *planetary model* of the atom in 1911

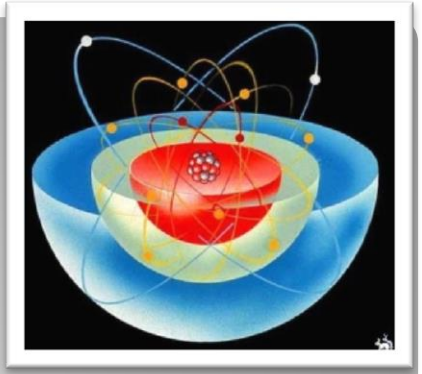




- **Niels Bohr,** 1913



THE STRUCTURE OF THE ATOM AND THE ELECTRON SHELL OF THE ATOM



- **An atom** is a complex electromagnetic system that includes elementary particles:

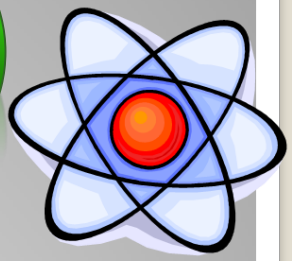
particle	designation	charge
Proton	p	+
Neutron	n	0
Electron	e	-

QUANTUM MECHANICAL THEORY CONTAINS TWO MAIN POINTS:

- *The electron has a dual nature. It has the properties of both particles and waves.*

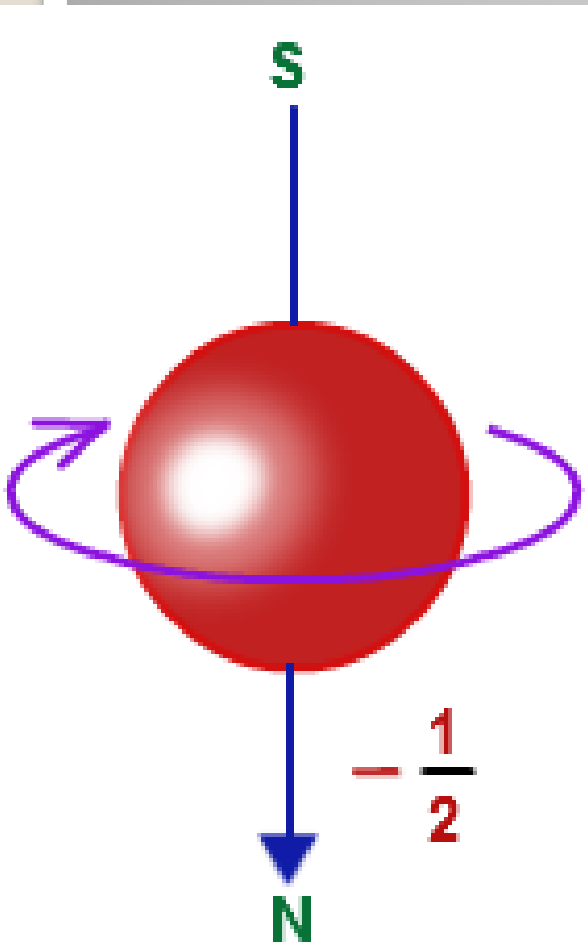
- *The position of the electron in the atom is uncertain.* We can't talk about any particular trajectory of the electron-we can only judge the degree of probability of its location at a given point in space.

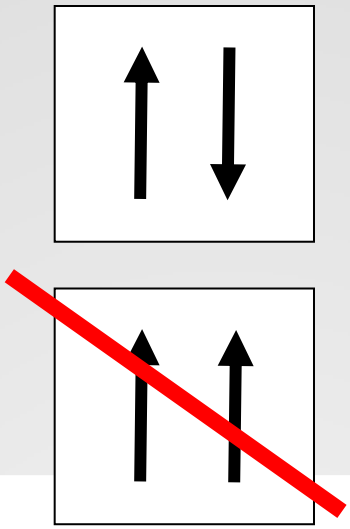
ATOMIC ORBITAL (AO)

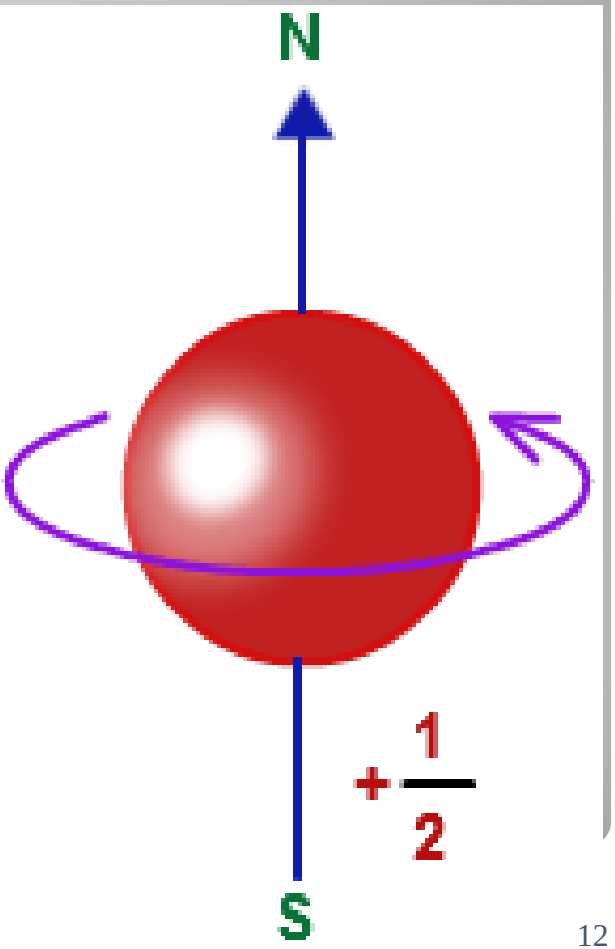


- **Atomic Orbital (AO)** this is the space around the atomic nucleus in which the probability of finding an electron is maximum.
- It follows that AO has certain spatial characteristics: **size, shape, and direction in space**, which are characterized by three quantum numbers: the main (n), side or orbital (ℓ), and magnetic (m).

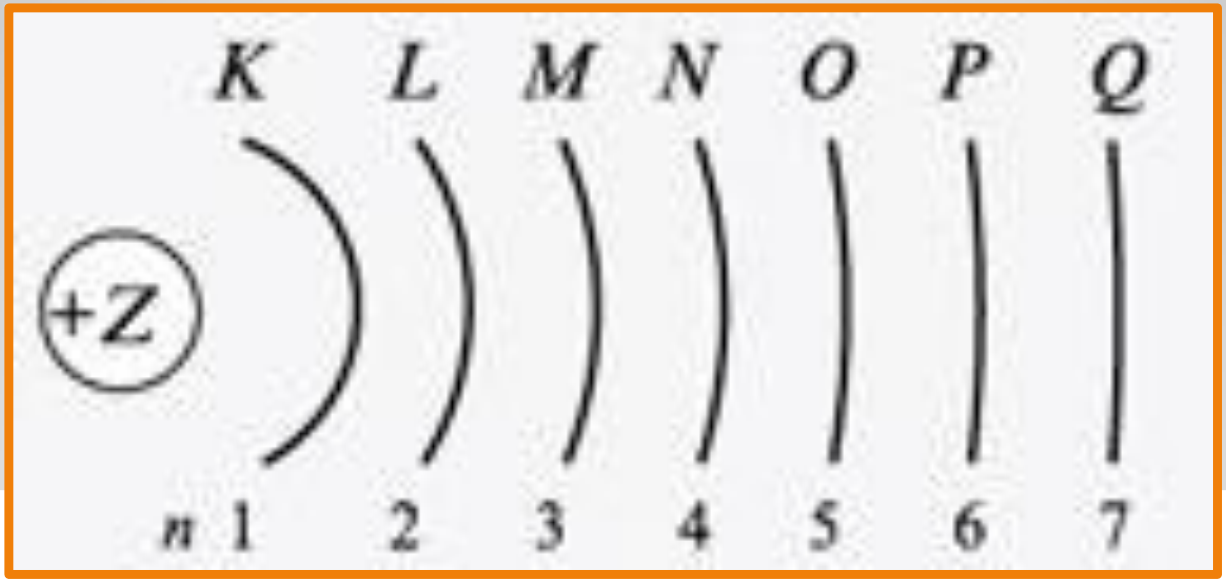
The spin quantum number (m_s)







- **1. The principal quantum number *n*** characterizes the remoteness of the AO from the nucleus (energy level). ***n*** takes integer values: ***n*** = 1, 2, 3, ..., which correspond to the number of the energy level (number of the period).



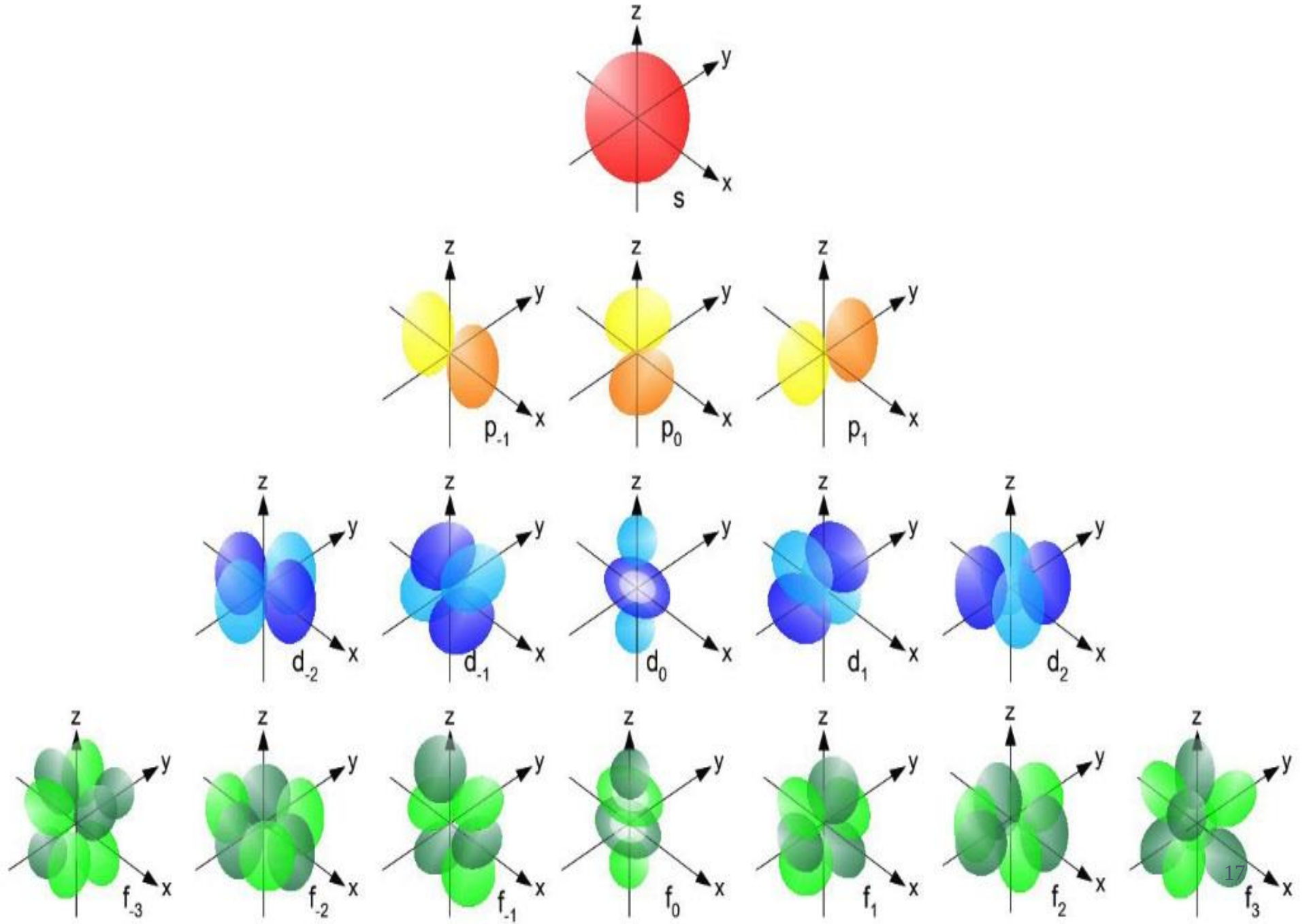
- **2. Orbital (side) quantum number *l*** characterizes the shape of atomic orbitals. ***l*** takes integer values from 0 to (***n*** - 1).
- ***n*** = 1**, *l*** = 0; the first energy level corresponds to the s-sublevel;
- ***n*** = 2**, *l*** = 0, 1; the second level has two sublevels: s and p;
- ***n*** = 3**, *l*** = 0, 1, 2; the third level - three sublevels: s, p and d;
- ***n*** = 4**, *l*** = 0, 1, 2, 3. the fourth and next levels - four sublevels: s, p, d and f.

value ℓ	Orbital shape
0	 s - orbital
1	 p - orbital
2	 d - orbital
3	 f - orbital

- **3. The magnetic quantum number** ***m*****$_l$** characterizes the direction of the orbital in space, that is, their number.

The magnetic quantum number ***m*****$_l$** can take integer values from **–*l*** to **+ *l***, including zero. ***m*****$_l$** determines the number of orbitals in the same electron layer:

1 s-orbital (m = 0),
3 p-orbitals (m = –1, 0, +1),
5 d-orbitals (m = –3, –2 , –1, 0, +1, +2, +3),
7 f-orbitals (m = –4, –3, –2, –1, 0, +1, +2, +3, +4)


z
y
x
s
p-1
p0
p1
d-2
d-1
d0
d1
d2
f-3
f-2
f-1
f0
f1
f2
f3

PRINCIPLES OF FILLING ELECTRONIC LAYERS

1) **Pauli's** principle
2) **Gund's** principle
3) The principle of least energy (**Klechkovsky's rule**)

The total energy of an electron is reflected by the sum of two quantum numbers: the main and the side **n + ℓ**. If for two orbitals the sum **(*n* + *l*)** has the same value, then the orbital with a smaller value of ***n*** and a larger value of ***l*** is first filled.

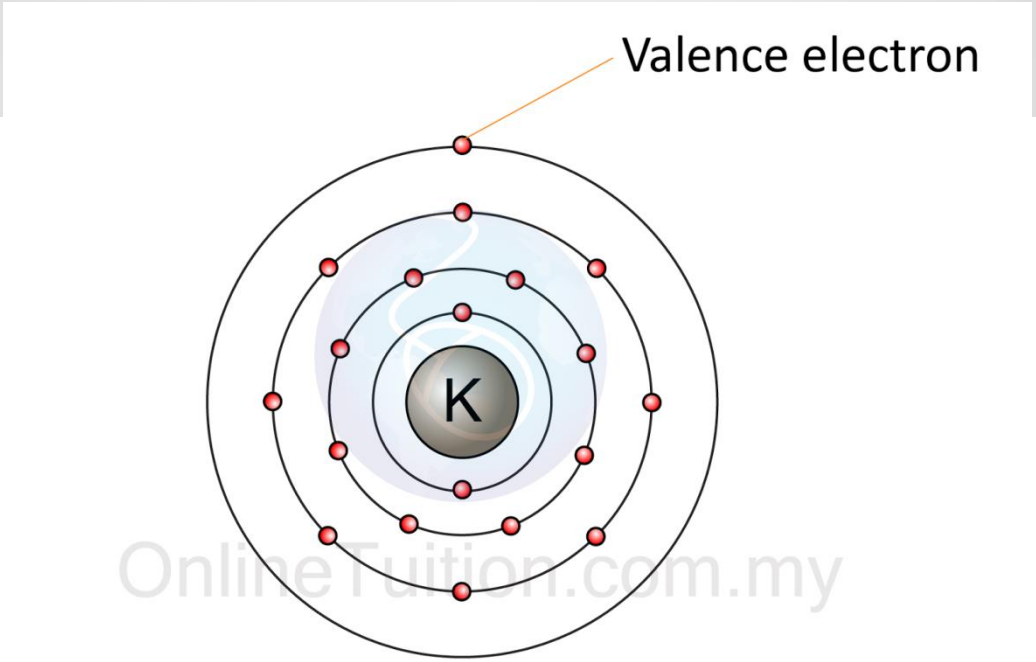
Accordingly, the orbitals can be arranged in a row in increasing energy:

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

The sequence of filling the orbitals of various electron layers with electrons can be imagined as follows:

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 5f^{14} 6d^{10}$$

Valence electrons



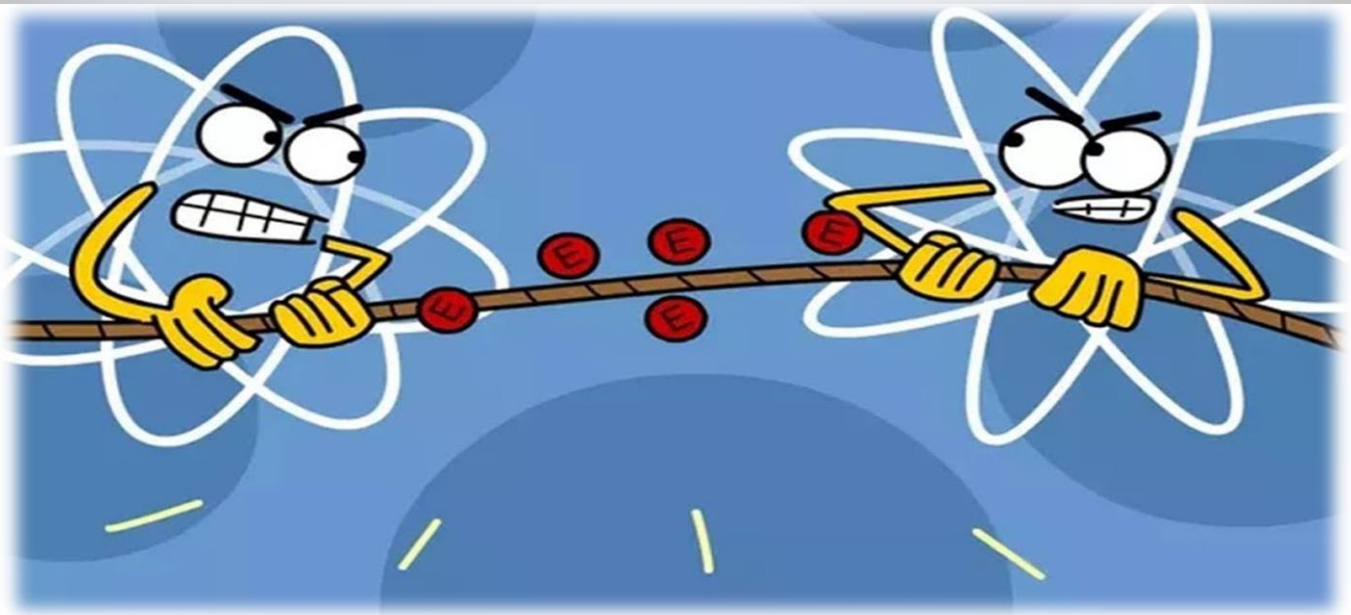
- **Valence electrons** are external level electrons for s- and p-elements, or external and incomplete pre-external sublevel electrons for d- and f-elements.
- ***These electrons determine the chemical properties of compounds.***
- ***These electrons are involved in the formation of chemical bonds.***
- Therefore, the electronic configuration of the valence level is the most informative and important for predicting the chemical behavior of elements.
- For elements of major subgroups, the number of valence electrons coincides with the group number in the Periodic table of elements.

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

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 \ldots$

s- elements	**s**	H **$1s^1$**; Be $1s^2$**$2s^2$**; Na $1s^2 2s^2 2p^6$**$3s^1$**	**$1s^1$** **$\ldots 2s^2$** **$\ldots 3s^1$**	**$1s^1$** **$\ldots 2s^2$** **$\ldots 3s^1$**
p- elements	**p**	B $1s^2 2s^2$**$2p^1$** Ne $1s^2 2s^2$**$2p^6$** P $1s^2 2s^2 2p^6 3s^2$**$3p^5$**	**$\ldots 2s^2 2p^1$** **$\ldots 2s^2 2p^6$** **$\ldots 3s^2 3p^5$**	**$\ldots 2s^2 2p^1$** **$\ldots 2s^2 2p^6$** **$\ldots 3s^2 3p^5$**
d- elements	**d**	Sc $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$**$3d^1$** Zn $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$**$3d^{10}$**	**$\ldots 4s^2$** **$\ldots 4s^2$**	**$\ldots 4s^2 3d^1$** **$\ldots 4s^2 3d^{10}$**
f- elements	**f**	Yb $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2$**$4f^{14}$**	**$\ldots 6s^2$**	**$\ldots 6s^2 4f^{14}$**

Chemical bonds



- The doctrine of chemical bonding (CB) is the central issue of modern chemistry. Without it, it is impossible to understand the reasons for the variety of chemical compounds, the mechanism of their formation, structure and reactivity. The formation of molecules from atoms leads to an energy gain, since under normal conditions the molecular state is more stable than the atomic one. The transition of a substance from an atomic state to a molecular state is caused by the occurrence of a (CB).

- An atom at the outer energy level can contain from one to eight electrons. If the number of electrons at the outer level of the atom is the maximum that it can accommodate, then this level is called **complete**. Completed levels are characterized by great durability. These are the outer levels of noble gas atoms:
- Helium (He) has 2 electrons on the outer level (s^2),
- the other noble gases have 8 electrons (ns^2np^6).

Why does a chemical bond occur?

1. Striving for the state with the lowest energy is a common property of matter. When molecules are formed from atoms, **the total energy of the system decreases.**
2. The desire of atoms to complete the outer electron shell, which is more favorable in energy. In chemical interactions, atoms tend to acquire a stable electronic configuration. According to the octet rule, the completed shell contains 8 e-ns^2np^6 (sum of 8), where n = 2,3,…

A CHEMICAL BOND is an electrostatic interaction between atoms involving valence electrons, accompanied by the release of energy (that is, a decrease in the total energy of the system). The formation of a chemical bond may lead to a rearrangement of the electronic configuration of the external level **(I group -** ionic, covalent, and metallic bonds**),** or it may not change this configuration **(II group -** hydrogen bonds and Van-der-Waals interactions**).**

A COVALENT BOND is a bond between two atoms of a non-metal using a common pair of electrons. The reason for the formation of a connection, as we noted earlier, is the desire to complete the configuration of its external level to an octet (8ē) or a doublet. The main characteristics of a covalent bond are its **energy and length, polarity and polarizability, multiplicity.**

General properties of a covalent bond

- **The bond length** is the distance between the centers of bound atoms.

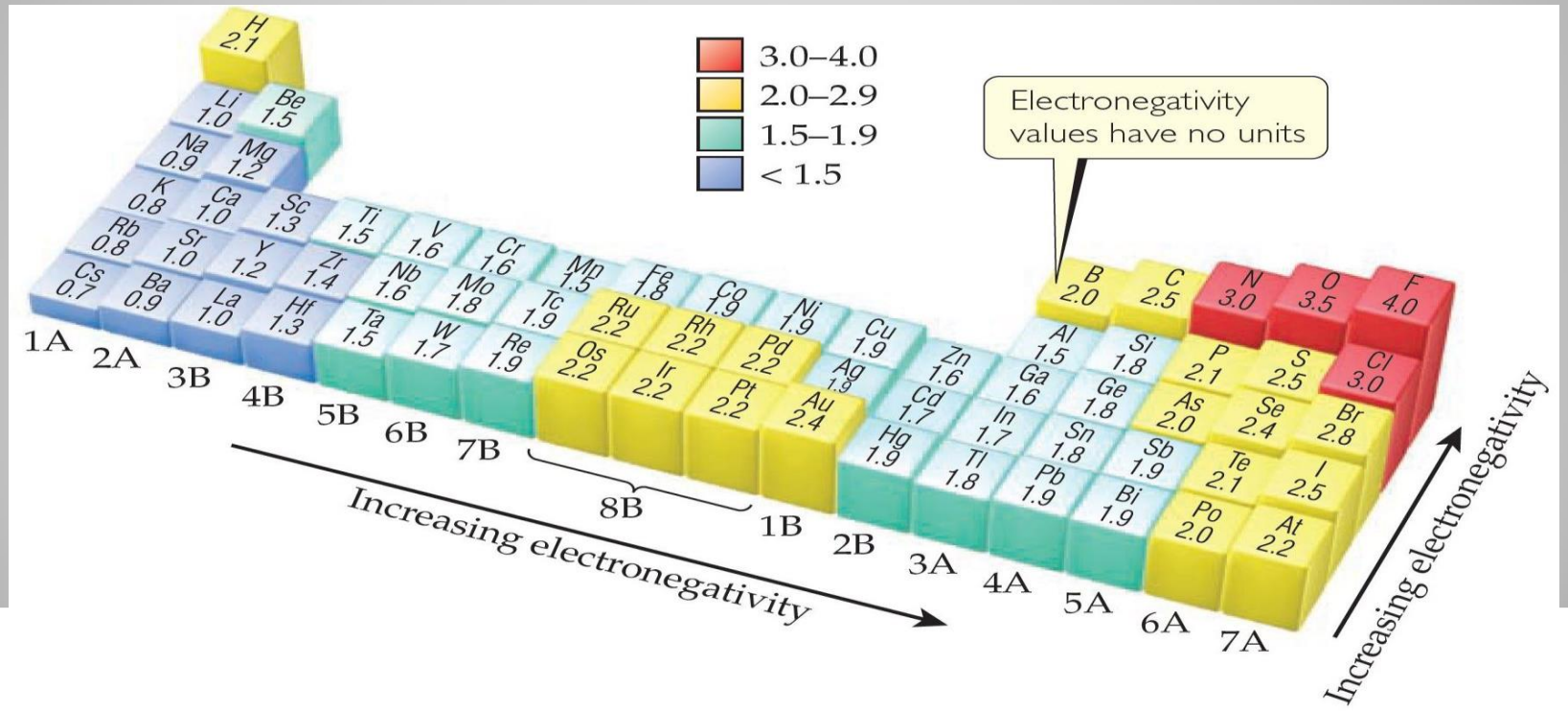
- For example, the bond lengths

C-C, C=C, and C≡C are

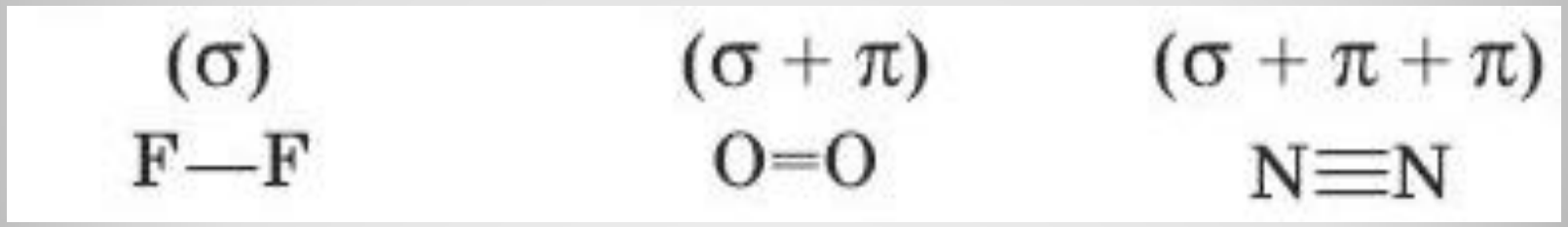
0.154, 0.134, and 0.120 nm, respectively

- **The bond energy** is the energy released when a bond is formed or required to break a bond. The system that contains less energy is more stable.

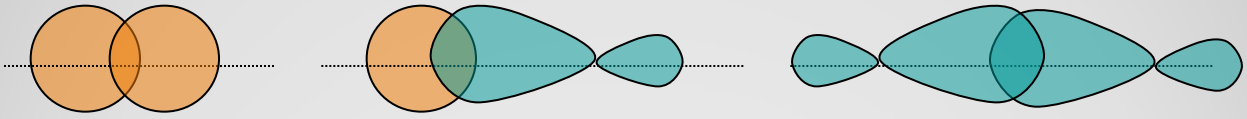
- **The polarity of the bond** is due to the uneven distribution of the electron density. The reason for the polarity is differences in the electronegativity of bound atoms.
- **Electronegativity (EO)** is the ability of an atom in a molecule to attract binding electrons. As the difference in electronegativity increases, the bond polarity increases.



- **Bond multiplicity** is the number of electron pairs socialized by neighboring atoms as a result of the formation of a covalent bond.
- In ethane, $H_3C–CH_3$ bond between carbon atoms is single, in ethylene, $H_2C=CH_2$ - double, in acetylene, $HC\equiv CH$ - triple.



- **The σ-bond** is formed when the atomic orbitals overlap axially and has an axis of symmetry that coincides with the line connecting the nuclei. The maximum electron density lies on this axis. All single bonds are **σ-bonds.**



s – s

H – H

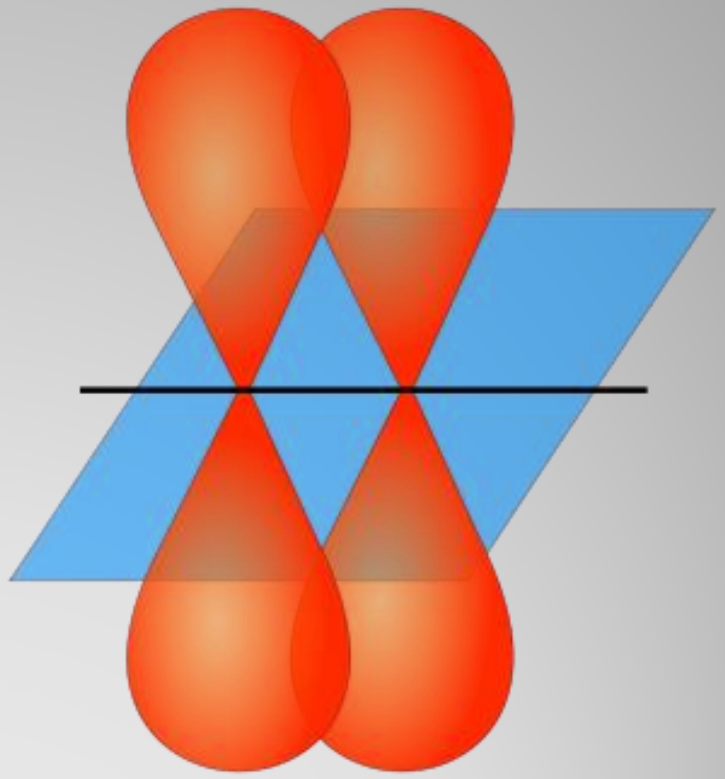
s – σ

H – C
H – N
H – O

σ – σ

C – C
C – N
C – O

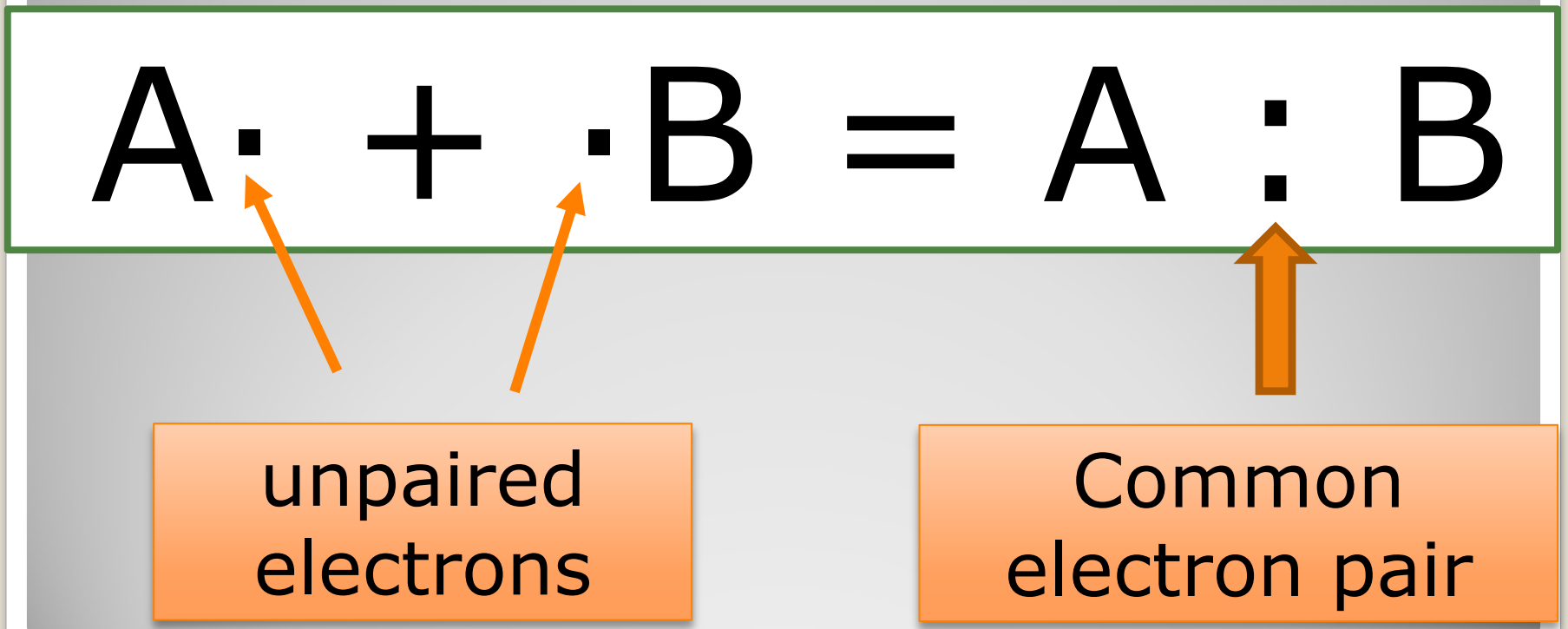
The π-bond is formed when the p-orbitals overlap laterally and has a plane of symmetry passing through the line connecting the atomic nucleus

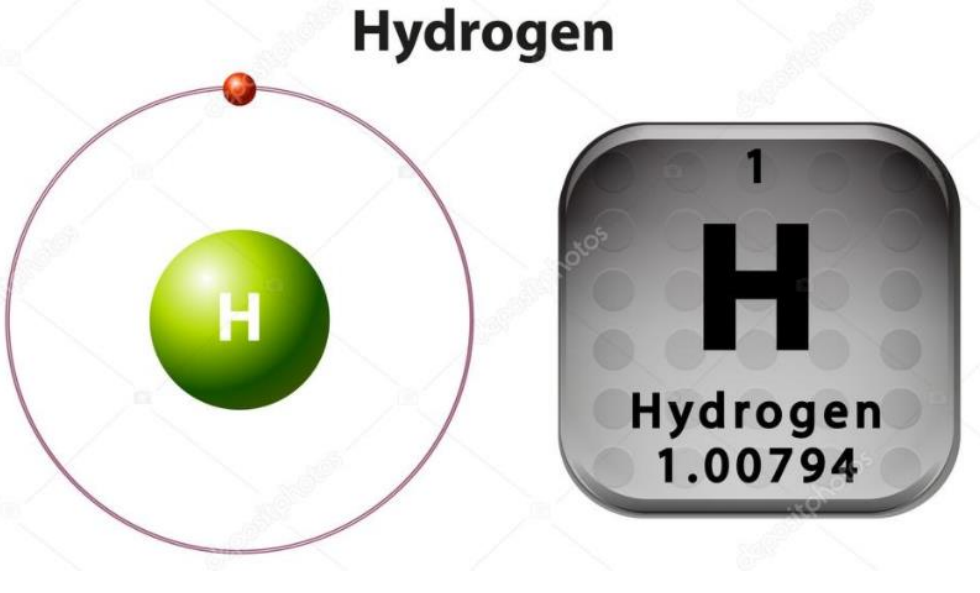


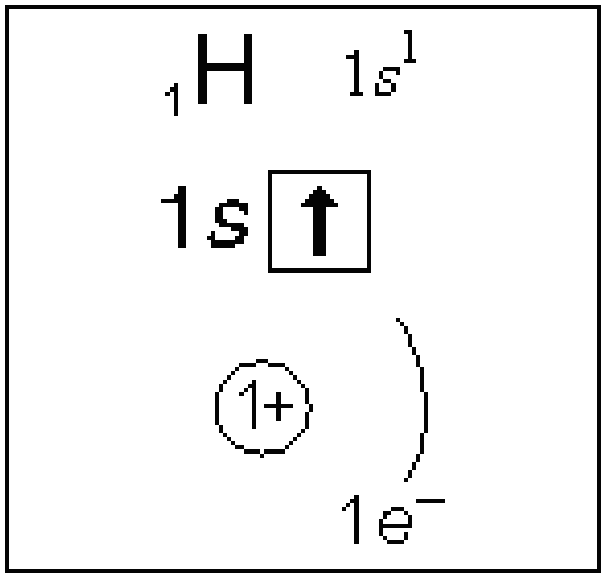
$(\sigma + \pi)$ $O{=}O$

$(\sigma + \pi + \pi)$ $N{\equiv}N$

The exchange mechanism







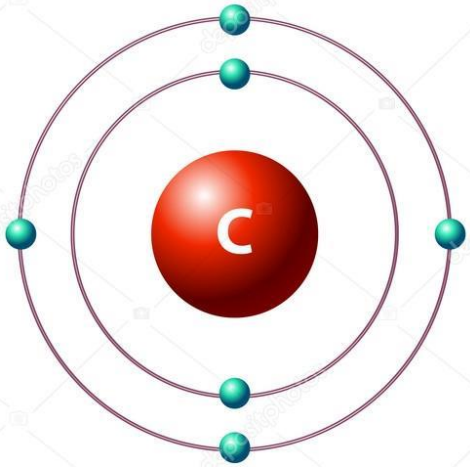
Electron Configuration of Hydrogen

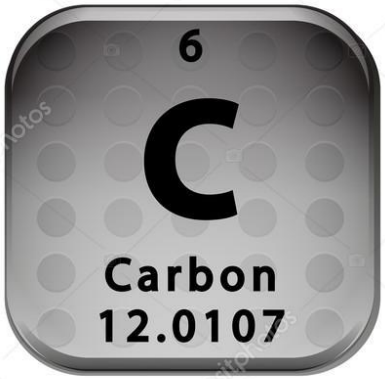
Energy Level

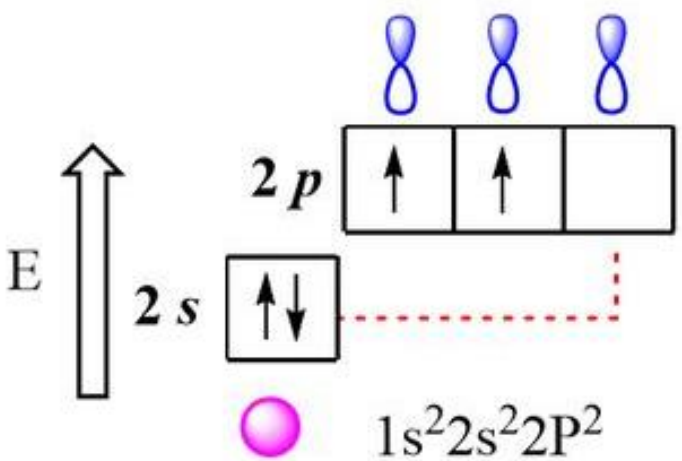
1 — Number of Electrons in This Orbital (Subshell)

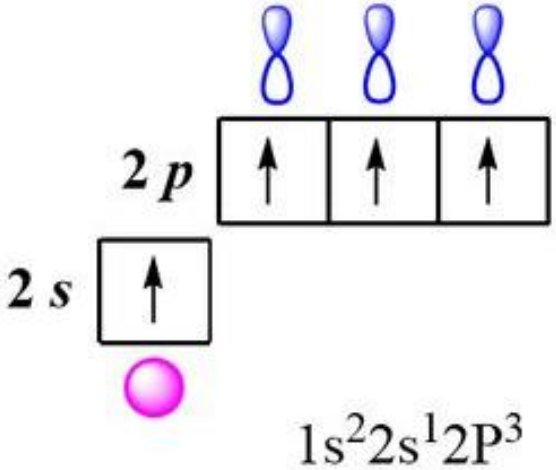
1s — Type of Orbital (Subshell)

Carbon





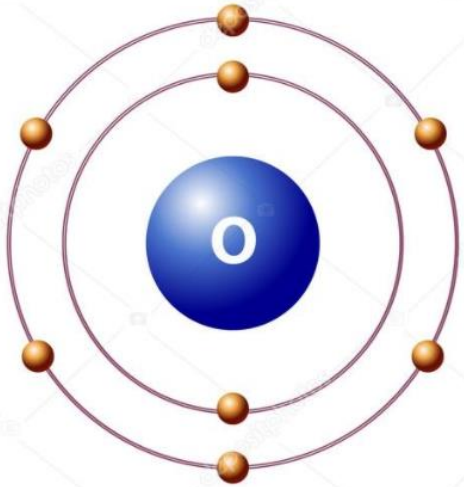


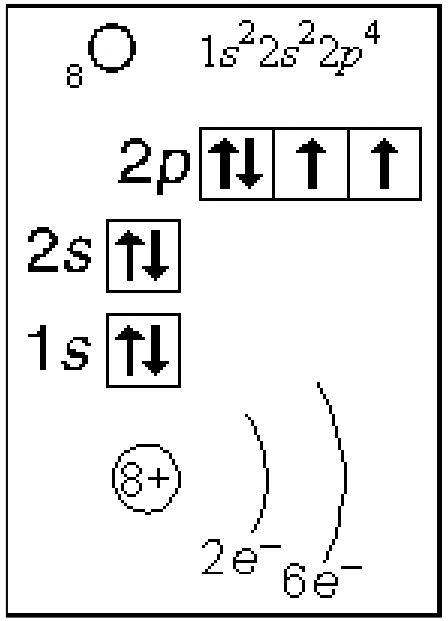


ground state for carbon

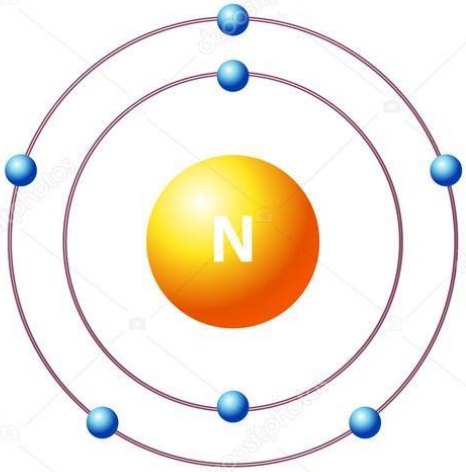
excited state for carbon

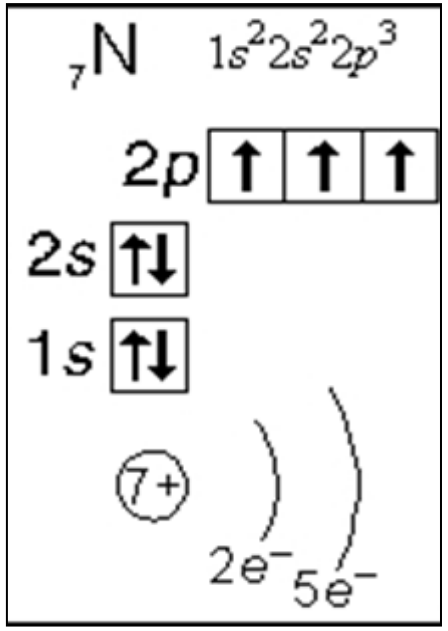
Oxygen



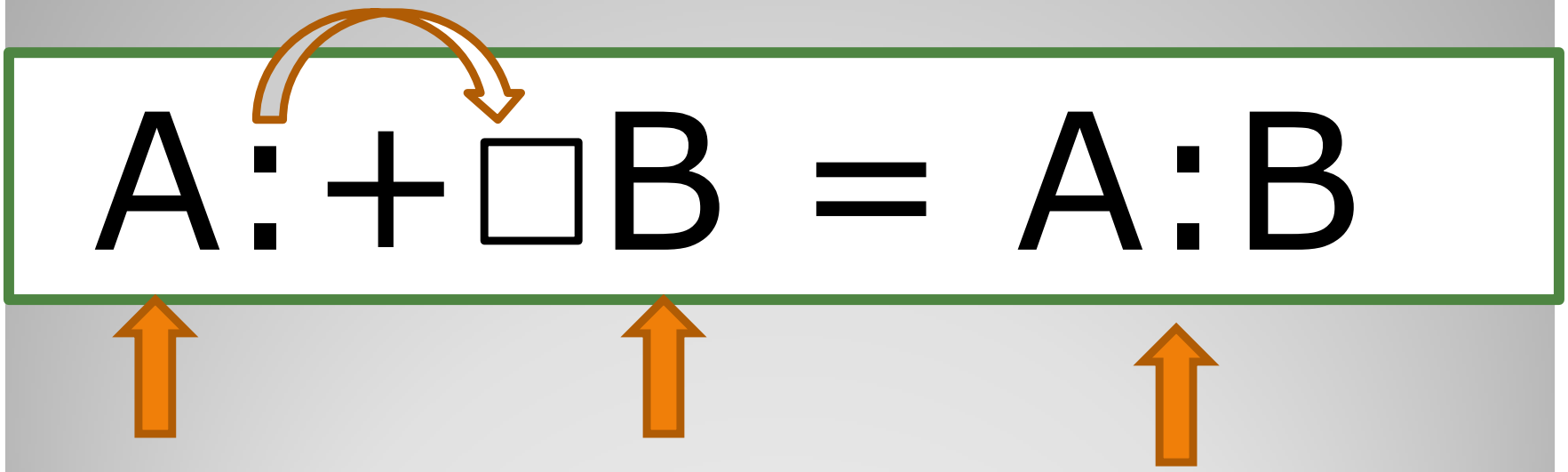


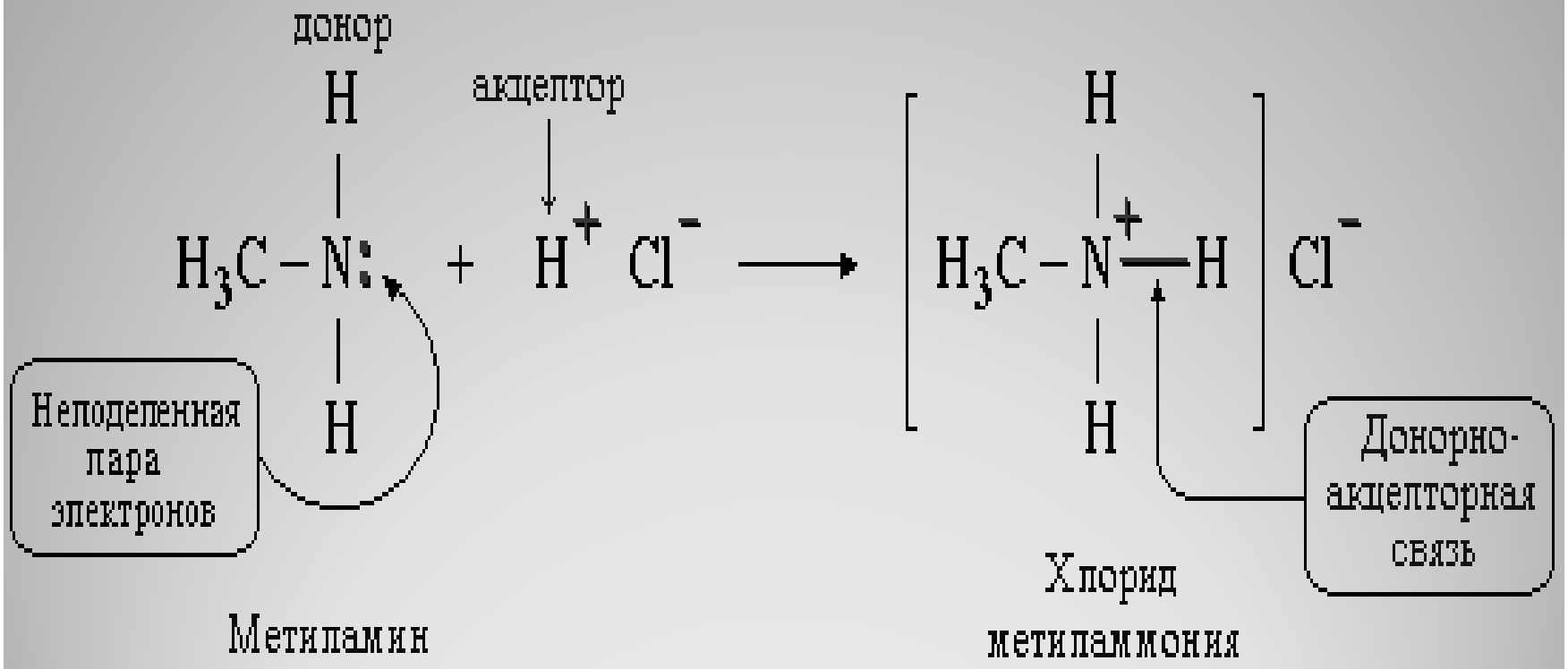
Nitrogen





The donor-acceptor mechanism




донор
акцептор
Неподеленная пара электронов
Донорно-акцепторная связь
Метиламин
Хлорид метиламмония

CONCLUSIONS

- Most of the biogenic elements are concentrated in the first three periods of the periodic table.
- By their position in the periodic table, one can find out the electronic configurations of the external and valence levels.