«Chemical Bond»

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* Lecture plan

1. General information about the chemical bond.
2. Covalent bond.
3. Ionic bond.
4. Metal bond.
5. Hydrogen bond.
6. Intermolecular bonds.

1. General information about the chemical bond

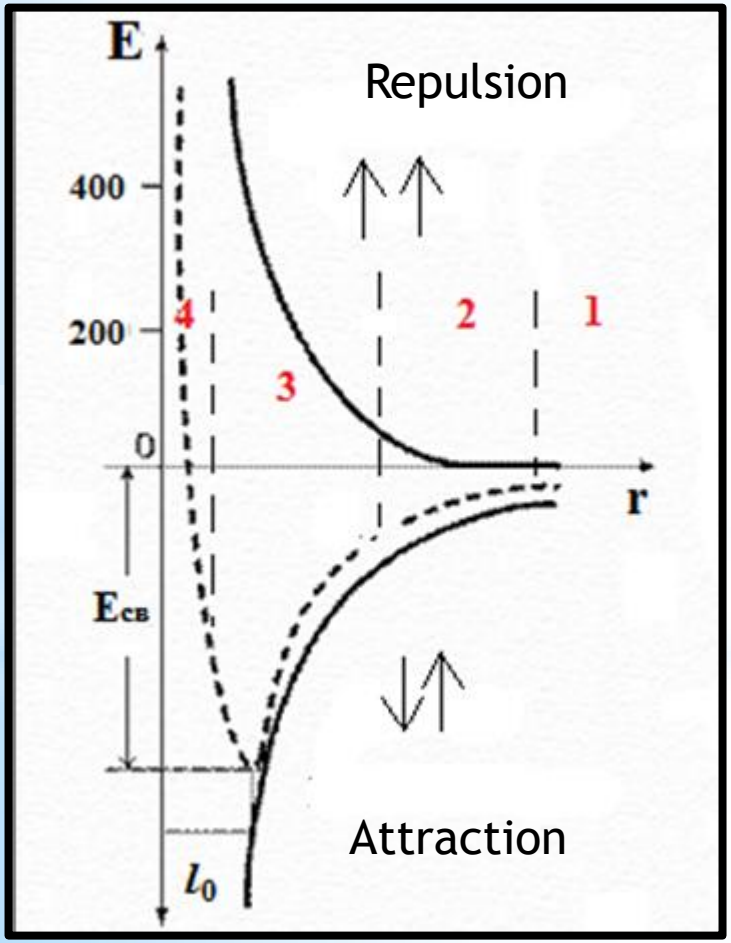
A chemical bond is any interaction between particles that releases more than 20 kJ of energy.

The main condition for the formation of **a chemical bond is a decrease in the total energy** of a polyatomic system compared to the energy of isolated atoms**.**

$$A + B = AB, \qquad E_{AB} < E_A + E_B$$

1. General information about the chemical bond

1927 Heitler and London calculated *E* and the *bond length* in the H_2 molecule using quantum mechanical calculations.



$E_{св}$ - chemical bond energy

l - bond length

1. General information about the chemical bond

Types of chemical bond

- Covalent
- Ionic
- Metal
- Hydrogen
- Intermolecular forces (van der Waals forces)

1. General information about the chemical bond

Characteristics

1) length ($\ell_{св}$) – internuclear distance between two chemically bonded atoms

- The **bond length** depends on the atomic radii:

	HF	HCl	HBr	HI
$\ell_{св.}$, нм	**0,092**	**0,128**	**0,142**	**0,162**

- The **bond length** depends on the multiplicity of the bond:

Bond	C−C	−C=C−	−C≡C−
$\ell_{св.}$, нм	**0,154**	**0,134**	**0,120**

1. General information about the chemical bond

2) Energy– energy spent on breaking a chemical bond, [kJ/mol]

The chemical bond is longer, the energy is less.

	HF	**HCl**	**HBr**	**HI**
$\ell_{св.}$, nm	0,092	0,128	0,142	0,162
$E_{св}$,kJ/mol	536	432	360	299

1. General information about the chemical bond

3) Valence angle – the angle between the bonds that form an atom in a molecule

Cl – Be – Cl ∠180°

H – O – H ∠104,5°

4) Chemical bond polarity – shift of electron density to a more electronegative atom

2. Covalent bond

- is a chemical bond formed by the atoms of two non-metals or Me and non-Me, provided $\Delta\chi$ **<1,8**.

E_{CB} = **100-800 kJ/mol**

There are two methods of Covalent Bond formation

such as

Valence bond method (VB)

Molecular orbital method (MO)

2. Covalent bond

Valence bond method

The unification of electrons occurs in such a way that an increased electron density arises between atoms in space, which ensures their connection.

2. Covalent bond

Basic postulates of the method of valence bonds

1. Interacting atoms can exchange electrons with each other, forming bonding pairs.
2. Two exchanging electrons must (Pauli's principle) have opposite (antiparallel) spins.
3. The bond is the stronger, the larger the area of overlapping atomic orbitals.
4. The overlapping atomic orbitals must be close in energy and symmetry.
5. Characteristics of a chemical bond (energy, length, polarity) is determined by the type of overlap of atomic orbitals.
6. The covalent bond is directed towards the maximum overlap of the atomic orbitals of the reacting atoms.

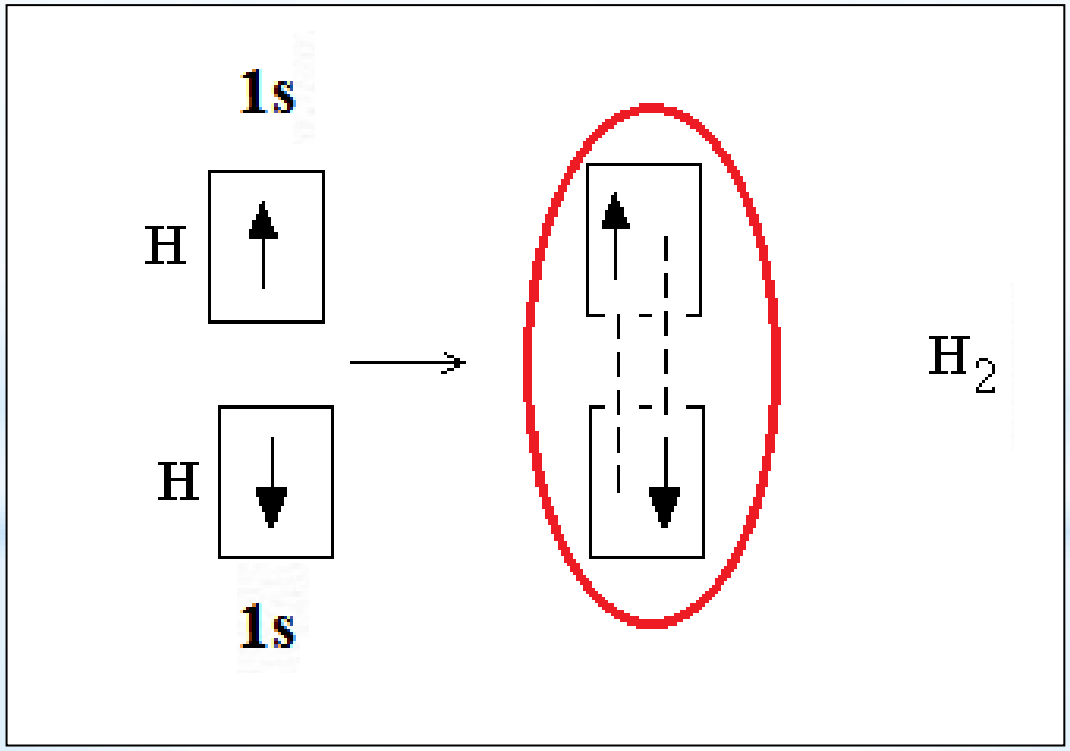
2. Covalent bond

Basic postulates of the method of valence bonds

1. The covalent bond is due to the formation of a common electron pair by sharing two electrons with antiparallel spins.
2. The covalent bond is two electronic, two-nuclear and localized.

2. Covalent bond

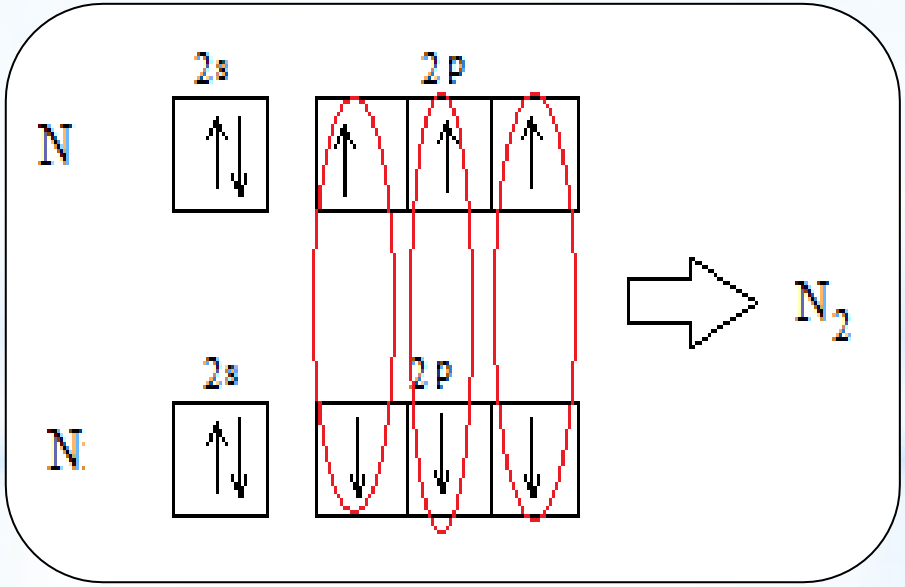
Formation of a covalent bond in a hydrogen molecule



2. Covalent bond

Mechanism of chemical bond formation

- exchange

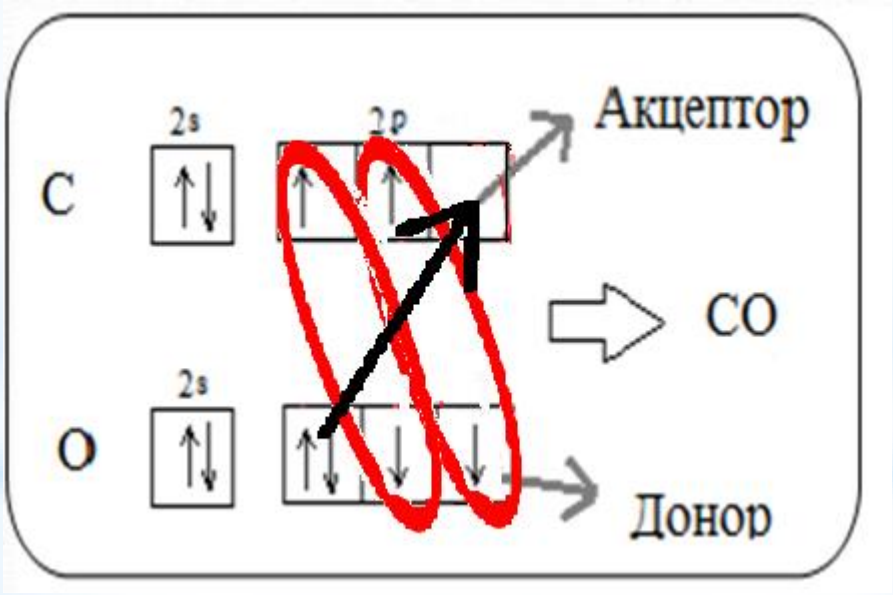


The multiplicity of the chemical bond is three.

2. Covalent bond

Mechanism of chemical bond formation

- donor-acceptor

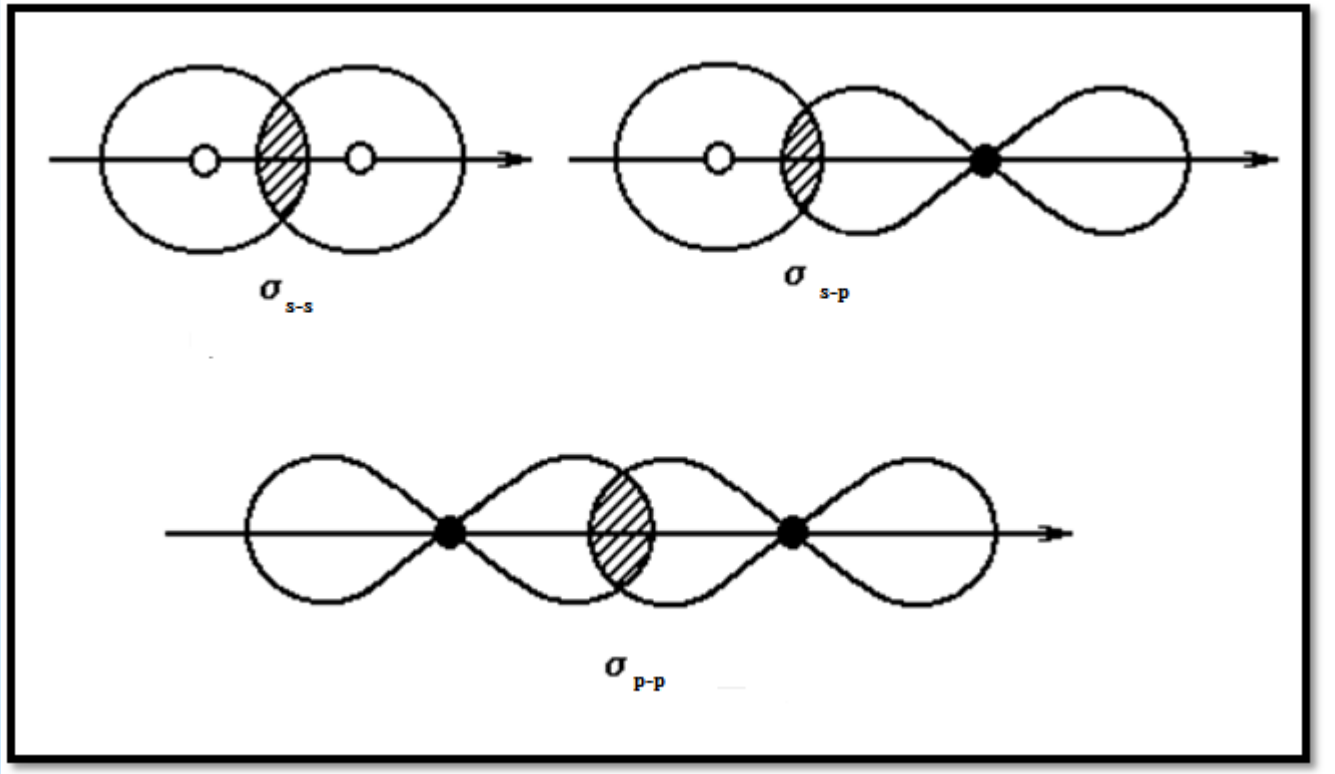


The multiplicity of the chemical bond is three.

2. Covalent bond

Overlapping electron clouds

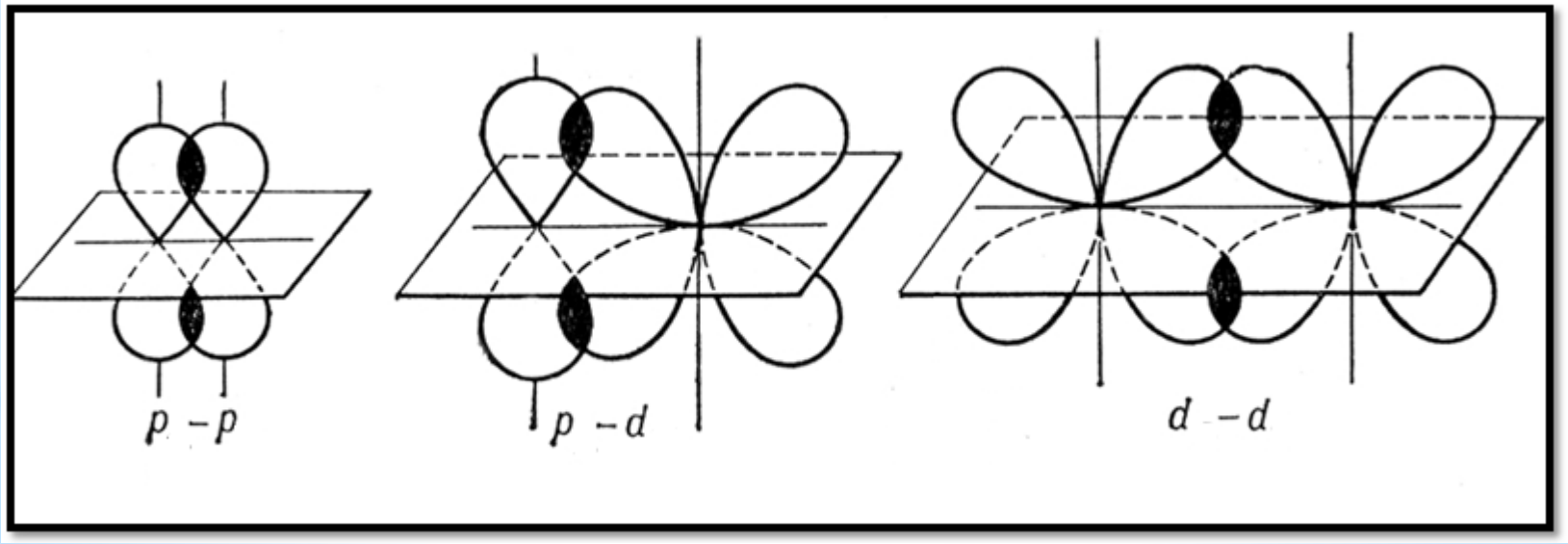
* σ – Bond (Sigma-bond): the area of the total electron density lies on the line of communication of the nuclei of atoms



2. Covalent bond

Overlapping electron clouds

π– Bond (Pi-bond): the area of total electron density is perpendicular to the bond line of atomic nuclei.



2. Covalent bond

PROPERTIES OF A COVALENT BOND

1. Polarity	is due to the uneven distribution of electron density due to differences in the electronegativity of atoms

Covalent bond

polar

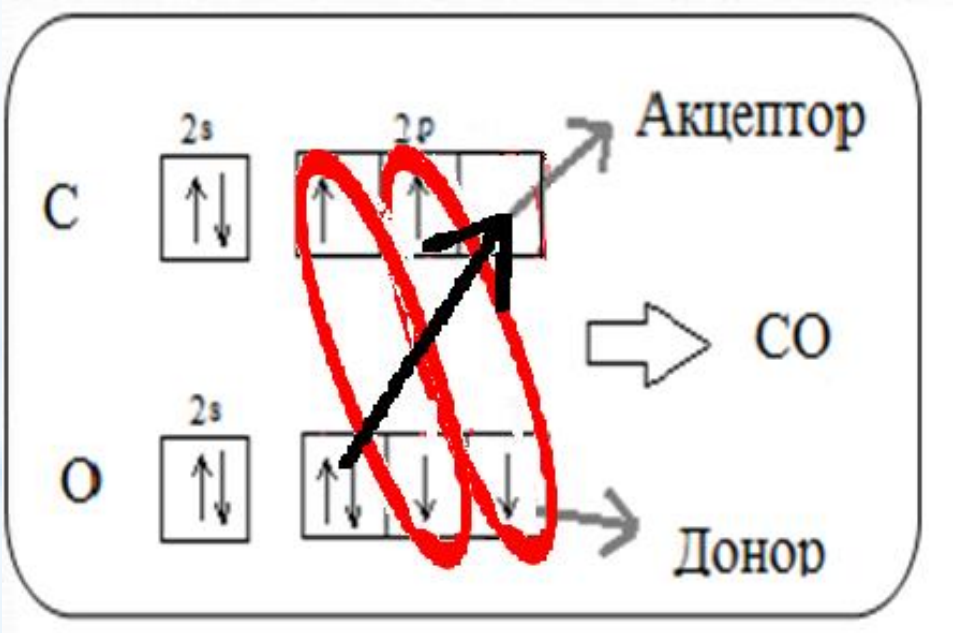
HCl, CO, H_2O

non-polar

H_2, O_2, N_2

2. Covalent bond

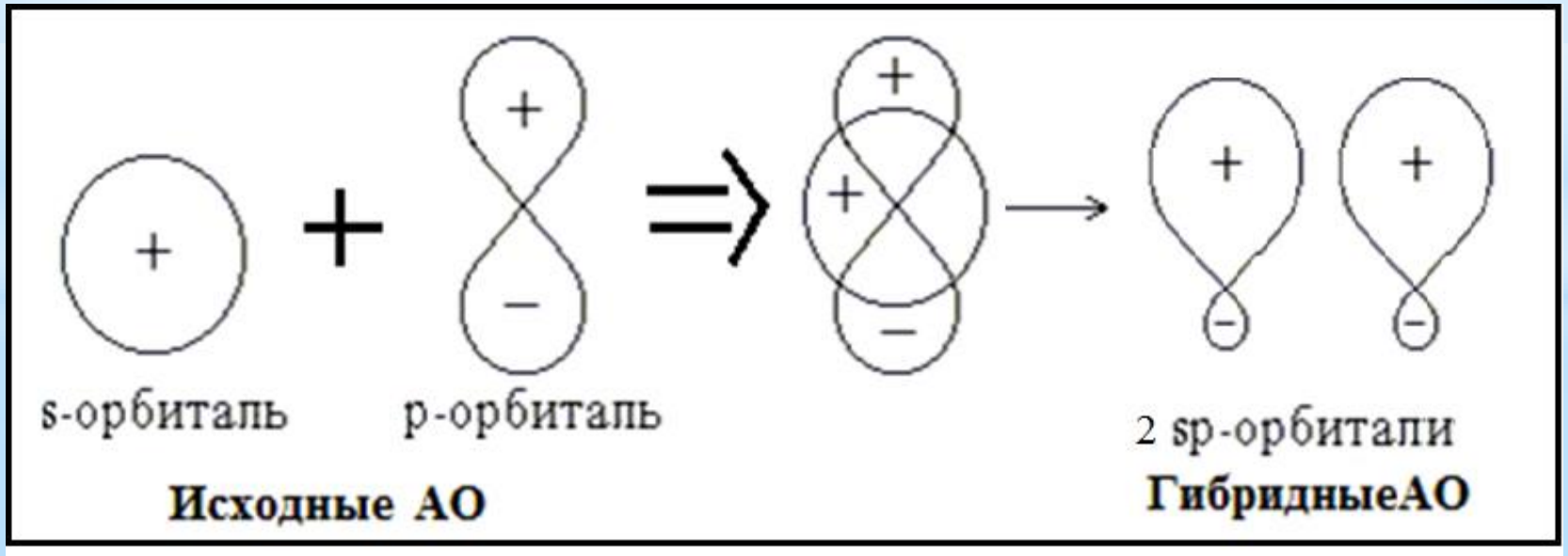
2. saturability	is the desire of atoms to fully realize their valence capabilities



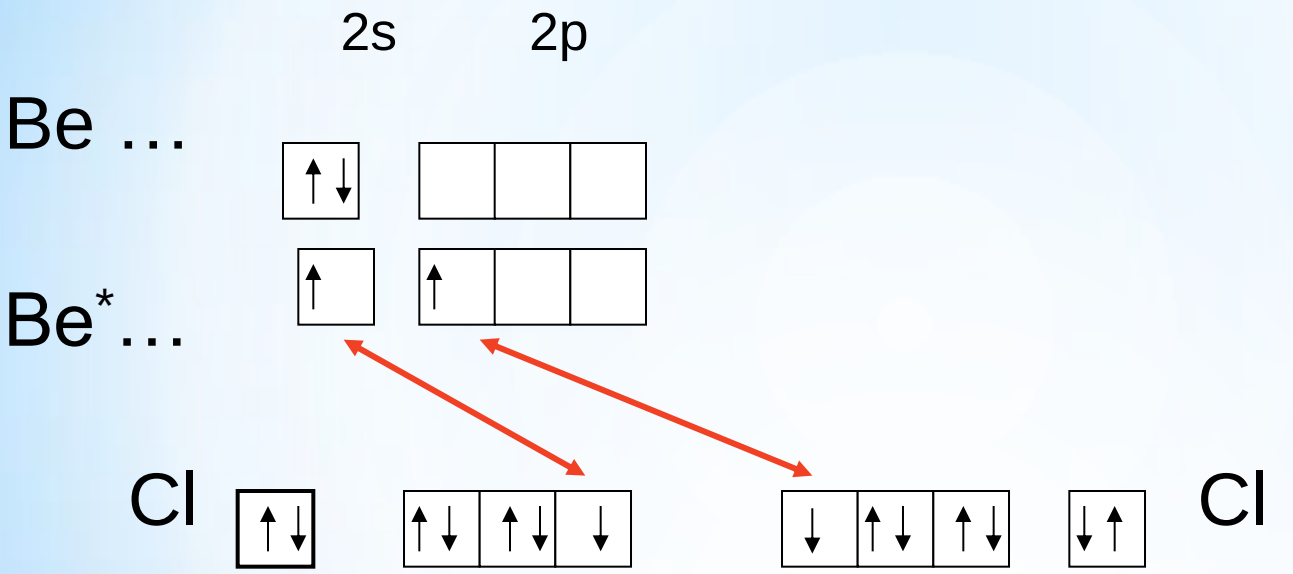
2. Covalent bond

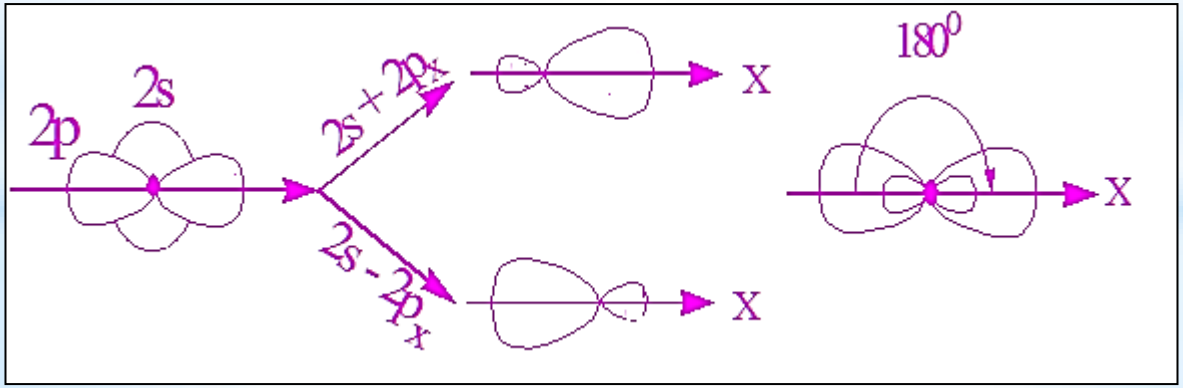
3. orientation	determines the geometric shape of molecules

Atomic orbital **hybridization** is the alignment of the shape and energy of atomic orbitals to achieve more efficient overlap.



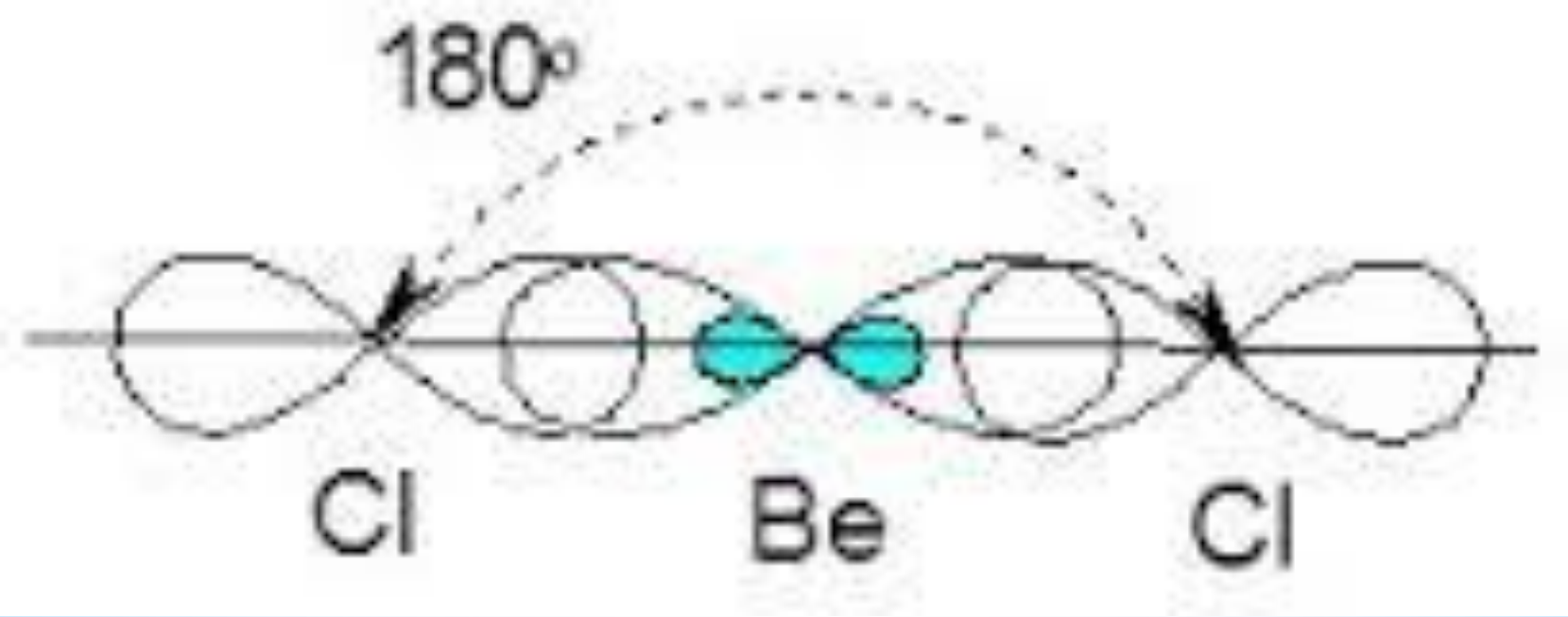
The structure of the molecule $BeCl_2$





Type of hybridization of atomic orbitals (Be) is sp.

Molecule structure is linear, angle is 180°


180°
Cl
Be
Cl

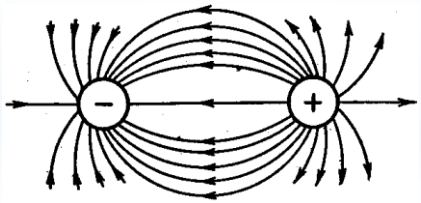
2. Covalent bond

Type of hybridization	**The geometric structure of the molecule**	**Valence angle**
sp	Linear	180
sp^2	Triangular	120
sp^3	Tetrahedral	109,28
sp^3d	Trigonal bipyramid	120 и 90
sp^3d^2	Octahedral	90

3. Ionic Bond

- formed due to electrostatic interaction between ions of the opposite sign.

The non-directionality of the ionic bond is due to the fact that the electrostatic field of the ion has spherical symmetry and it is able to attract ions of the opposite sign in any direction.



Unsaturation is the ability of an ion of a given sign to attract a variable number of ions of the opposite sign.

3. Ionic Bond

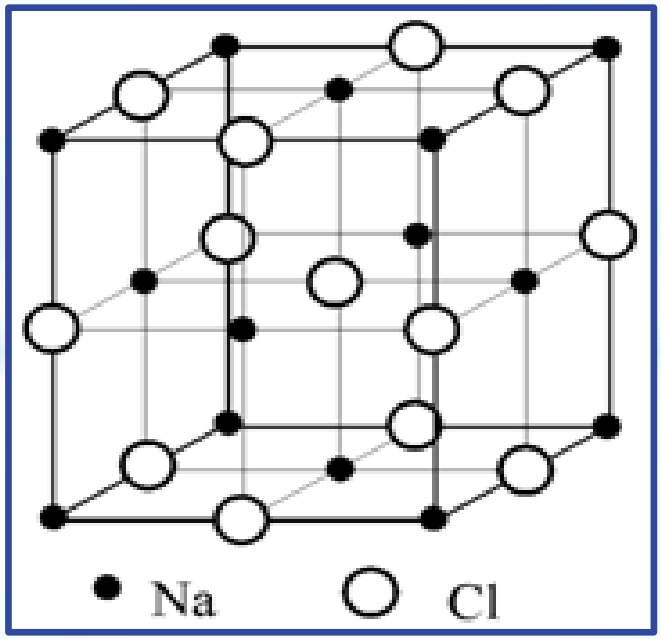
With a difference in the electronegativity of atoms

$\Delta\chi$ **>1,8** (on the Pauling scale) is an ionic bond,

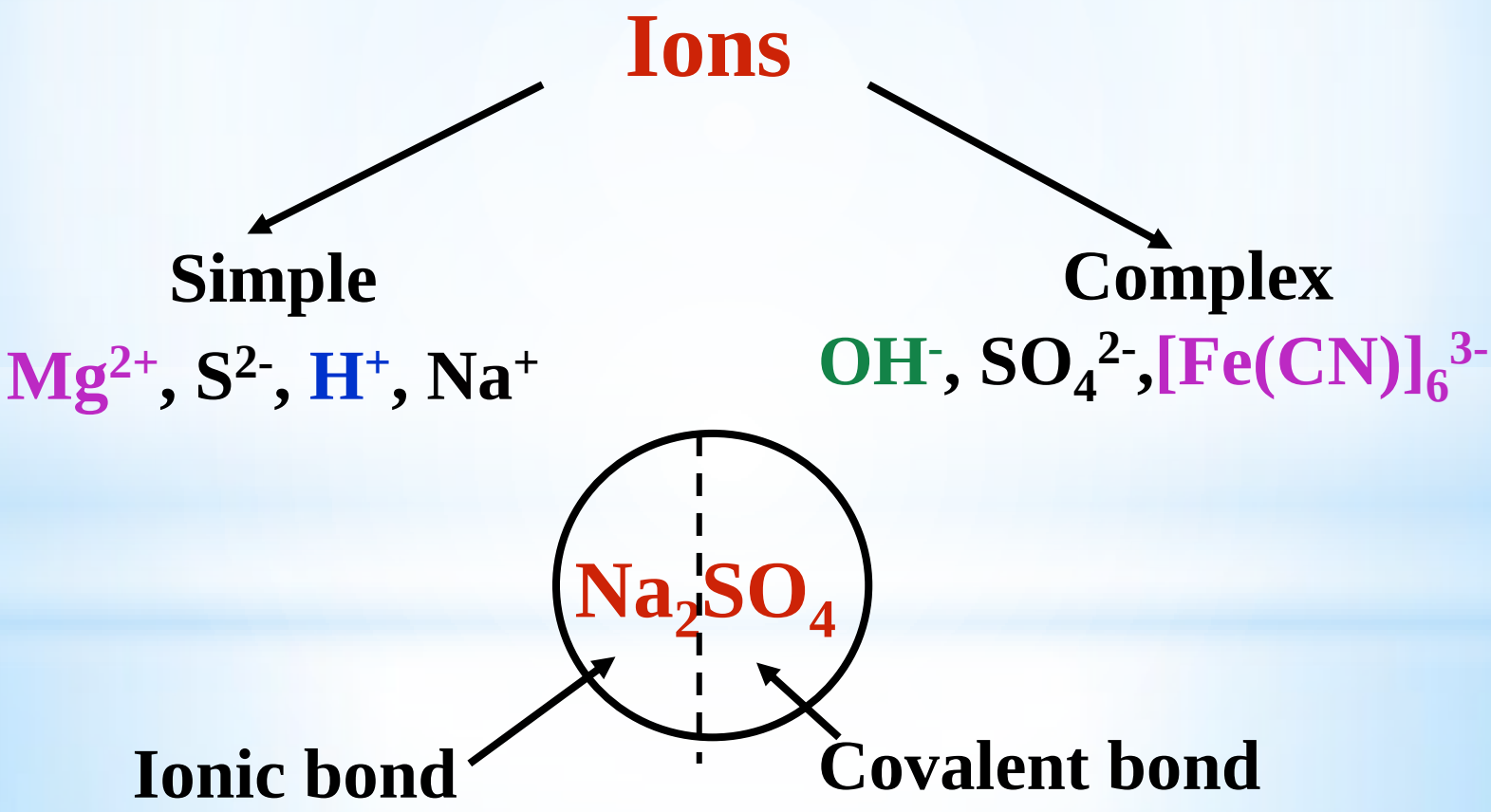
$\Delta\chi$ **<1,8** – covalent bond.

NaCl

$\Delta\chi$ = 3,0 (Cl)- 0,9 (Na) = 2,1



3. Ionic Bond


Ions
Simple
Mg^{2+}, S^{2-}, H^{+}, Na^{+}
Complex
OH^{-}, SO_4^{2-}, $[Fe(CN)]_6^{3-}$
Na_2SO_4
Ionic bond
Covalent bond

3. Ionic Bond

* At ordinary temperatures, ionic bonds exist in the solid state.

* Ionic crystals have high melting and boiling points.

* Ionic crystals melt with increasing volume.

* Compounds with an ionic bond are highly soluble in water, their solutions are electrically conductive.

4. Metal bond

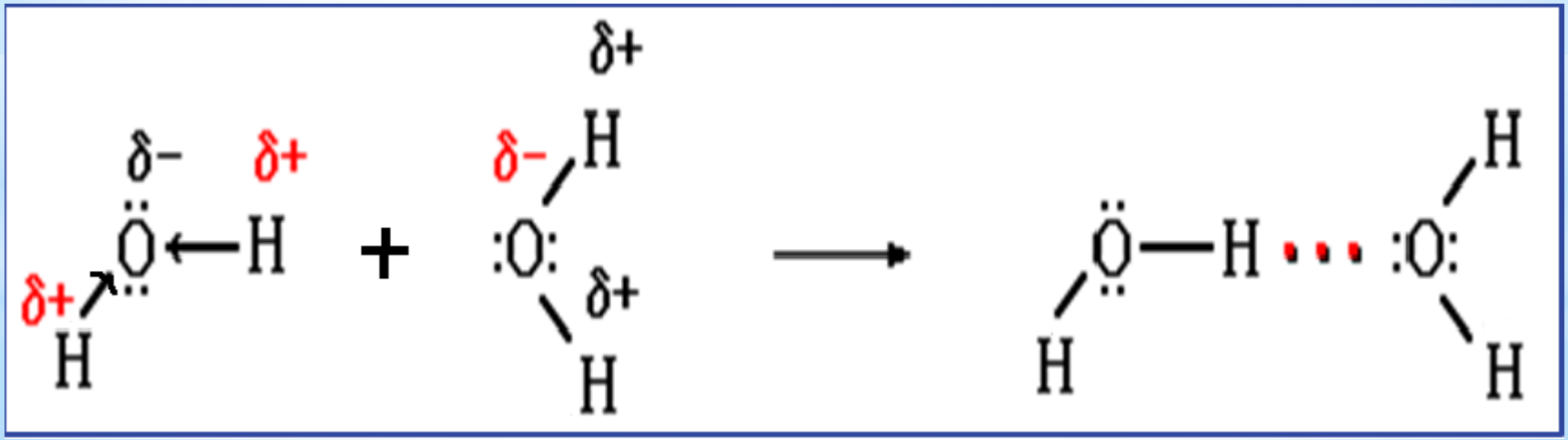
- formed by the interaction of positive metal ions and valence electrons, as well as between atoms

$E_{св}$ =100-200 kJ/mol

5. Hydrogen Bond

- occurs in molecules or between molecules, which include a hydrogen atom and the most electronegative atom (F, O, N).

$E_{св}$ = **20-40 kJ/mol**



5. Hydrogen Bond

The presence of hydrogen bonds affects the properties of substances:

1. Substances are made up of associated molecules.
2. The density of a substance increases during the transition from a solid to a liquid state (water).
3. Substances have higher boiling and melting points.

6. Intermolecular chemical bonds

Type	Definition	Examples
Dispersion	interaction between two nonpolar molecules	H_2 и N_2, H_2 и H_2
Induction	interaction between two polar and nonpolar molecules	HCl и O_2, NH_3 и N_2
Orientation	interaction between two polar molecules	HCl и HCl HBr и HCl

Home task № 1.

1. Please, determine the type of chemical bond in substances: copper, sulfuric acid, sodium hydroxide, oxygen molecule, water, ammonia, potassium bromide

Home task № 2.

1. Please, show the formation of a methane molecule (CH_4) by the method of valence bonds, determine the shape of the molecule.