Āris Kaksis 2019 Year, **Riga Stradin`s University**: http://aris.gusc.lv/BioThermodynamics/4KimiskaSaiteAngl.pdf

Chemical interaction forces and covalent bond

Interaction forces between atoms, ions and molecules are absent just in gas state of substances. If cool gases enough its becomes liquid and freeze solid, because between atoms, ions and molecules are forming chemical interactions forces, due to interaction forces particles stick together and aggregates.

Chemical interaction are attraction and binding forces, what works between atoms, ions and molecules, forming compounds, aggregates and complexes. In nature it can observe as atoms, molecules and ions attracts and stick together, for example: water vapors (gas water molecules H_2O) forms rein drops, snowflakes , fog and clouds, which merge and precipitate getting into puddles, lakes, rivers, sees, oceans, glaciers and snow coats. Chemical binding forces according its strength are classified as weak chemical interaction forces, as moderate chemical interaction forces and as strong chemical interaction forces, where strong interaction forces are called as **chemical bond**. **Chemical bond establishes between two** atoms according exchange mechanism or donor-acceptor mechanism.

1. Exchange mechanism binds two atoms with common binding electron pair orbital [↓↑] [N S ↑↓ S N], what has the name **covalent bond**. That forms commonly for two atoms, if one atom on outer electron shell energy level has single unshared electron with spin N↑s $+^1/_2$ [↑] and, if second atom on outer electron shell energy level has single unshared electron with opposite spin S↓N $-^1/_2$ [↓]. That binds chemical bond members, atoms firm together with single value chemical **covalent bond** between atoms. From primary school is known, that **covalent bond** to each of two atoms make in chemical compound one **valence value**. Total **valence** number for chemical element atom in compound determines this atom made number **of covalent bonds**.

2. Donor acceptor mechanism binds two atoms with common binding electron pair orbital [↓↑] , what has the name **donor-acceptor bond** or **coordinative bond**. That forms commonly for two atoms, if one **central atom** on outer electron shell energy level has empty orbital [ ] , and, if second atom on outer electron shell energy level has at least one unshared electron pair orbital [↓↑]. **Central** metal element **atom** usually is **cat ion** with empty several orbitals [ ] , in which atom **acceptor coordinates** around itself one, two, four or six atoms, which are electron pair **donors** [↓↑], and those call as **ligands**. In **coordinative compound** central atom has **coordination number**, which corresponds to **donor-acceptor bond** number, donor atom account and **ligands** number, which coordinates around **central atom**.

VSEPR Valent Shell Electron Pair Repulsion according Exchange Mechanism.

Chemical bond between two atoms makes common electron pair, what call as **covalent bond**.

Covalent – *co* in *Latin* – common, with and – *valēre* in *Latin* – to be valuable.

Chemical interaction problem, binding with **covalent bond** or any other **chemical interaction bond** is science central problem.

I , II , III Covalent bond types in chemistry and examples

I Covalent *nonpolar*, *polar* , *ionic* **bond**: nonmetals, oxides, acids, bases, salts, minerals, organic compounds;
II Donor-acceptor bonds or **coordinative bonds: complex** or **coordinative compounds** and

III. **Metallic bond in metals** are for **s** orbital electrons [↑] [↓] which have saved free, spherical ground wave state in body of **metals** and as the free electrons in **metals** assign for its **metallic** properties : reflect the light as mirror, conductivity etc. as for example: Al, Fe, Cu, Ag, Au, Pt etc..

Different in **nonmetal** [↑] [↓] **p**, [ ] **d** and **f** [ ] orbitals electrons are localized at node planes and can not be free on positive charged atom nuclei, which site is localized on node plane, as it is obviously observing opposite to free electrons on **s** orbital [↑] [↓] electrons in **metallic** body, which do not have node planes and as well as are in **metallic** body free electrons,
as well as electrons **s** are independent on atomic nuclei because of node plane absence and
as well as belong to all atoms of **metallic** body instantly.

Exchange mechanism - σ, π covalent bonds.

Valent Shell Electron Pair Repulsion (VSEPR) according exchange mechanism define fife points, what reveal covalent bond properties to form non polar, polar and ionic covalent bonds, which have the compounds

nonmetals, oxides, acids, bases, salts, minerals and organic compounds

1. Covalent bond bind both atoms with common **electron pair** having opposite spins .

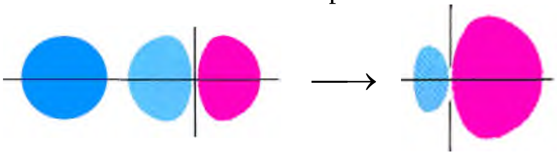
1. atoms 2. atoms

• ↑↓ •

2. Electron pair establish **overlapping** both orbitals. If stronger is **overlapping**, then stronger is **covalent bond**.

Hydrogen **1s** [↑] orbital and fluorine **2p** [↓] orbital overlapping between atoms make common electron pair orbital [↓↑] – **covalent bond** (1.figure)

↓ node plane ↓ of fluorine atom



designation of chemical formula using different types:

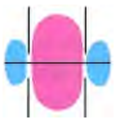
H + **F** ⟶ **H-F** **Structural formula** **Electron formula** **Molecular formula**

H[↑] + [↓]**F** ⟶ **H**[↓↑]**F** **H—F** **H** $\overset{+}{\cdot}$ **F** (: : :) **HF**

1.Figure. **Covalent bond** formation between **H** and **F** atoms **overlapping** electron orbitals. Common electron pair [↓↑] of both atoms valent electron adding [↑] + [↓] with opposite spins.

3. Orbital **overlapping zone** between positive charged **(+)** nucleus increased electron negative charge **(—) density** weaken repulsing forces between atoms and strengthening **covalent bond**.

node planes ↓ ↓ of chlorine atoms



designation of chemical formula using different types:

Cl—Cl **Structural formula** **Electron formula** **Molecular formula**

Cl^{+}**e**$^{-}$[↓↑]**e**$^{-}$**Cl**$^{+}$ ⟶ **Cl—Cl** $^{+}_{+}$**Cl** $\overset{+}{\cdot}$ **Cl** (: : :) chlorine molecule Cl_2

2.Figure. Electron negative ↑ **(—)** charge **density** between positive charged **(+)** nucleus weaken repulsing forces and strengthening **covalent bond**.

4. Covalent bond is **saturated**, because common orbital of both atoms may occupy just two electrons with anti-parallel spins [↓↑]. Any chemical element atom valence in compound is univalent and corresponds to one common orbital with two electrons [↓↑]. Hydrogen in compounds is univalent **H-H** (**H:H** hydrogen molecule H_2), **H—O—H** in water molecule H_2O hydrogen is univalent. Oxygen **—O—** is two valent with two **valences** – each of two **covalent bonds** is **saturated** **H**[↓↑]**O**[↓↑]**H** having valence one whole.

5. Covalent bond has central atom **symmetric geometry in space**, what optimize maximal **overlapping orbitals** along chemical bond between atoms. Atoms bind to form central **symmetric geometric figures**, which forming with **valence angle** and **bond length** (distance between atoms).

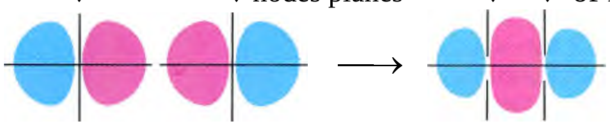
http://aris.gusc.lv/BioThermodynamics/CrystalloGraphy.pdf

Molecular orbitals (covalent bonds) are forming two possible types of orbital overlapping configuration sigma σ (singular) bonds, which apply symmetrisation around central atom,

http://aris.gusc.lv/BioThermodynamics/CrystalloGraphy.pdf and pi π (paired) bonds.

3.fig. F-F σ bond forms p orbitals which symmetry axes align on one line. Orbitals approaches with electron anti parallel spins and fuse in **red** region, blue regions remain outside behind atom nuclei. Nodes planes retain position on atom nuclei perpendicular to symmetry axes and are correlated parallel each to other.

↓ ↓ nodes planes ↓ ↓ of fluorine atoms



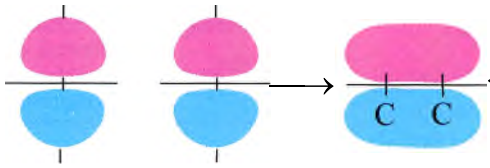
designation of chemical formula using different types:

F [↑] + [↓] **F** ⟶ **F** [↓↑] **F** **Structural formula** **Electron formula** **Molecular formula**

F + **F** ⟶ **F—F** $^{++}_{++}$**F**:**F**: fluorine molecule $\mathbf{F_2}$

3.Figure. **F** and **F** atomic p orbitals fuse into σ molecular orbital and form electron negative charge **(—) density** between fluorine positive charged atom nuclei weakened repulsion forces and strengthening covalent bond in fluorine molecule $\mathbf{F_2}$. Atomic nuclei lies on parallel orbital node plans perpendicular symmetry axis line, which divide negative charged electron (—) density into three symmetric regions and greatest electron density lies between atomic nuclei.

node plane →



←on node plane lie both carbon atom nuclei

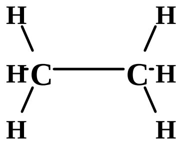
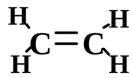
C + **C** ⟶ **C—C** ⟶ >**C=C**< double bond with σ and π bonds

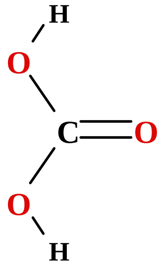
C [↑] + [↓] **C** ⟶ **C** [↓↑] **C**

4.Figure. **C** and **C** atomic orbitals fuse into π molecular orbital and form in double bond >**C=C**< second bond after sigma σ bond **C—C** formation. On common node plane lie both carbon atomic nuclei, but negative charge **(—) density** between positive charged atom nuclei weakened repulsion forces and strengthening covalent bond together with sigma bond σ on formed double bond >**C=C**< .

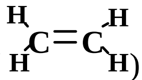
π bond forms overlapping (**C** and **C** or **O** or **S** or **P** or **N**) atomic electron orbitals with parallel symmetry axis. Atomic nuclei approach on common node plane and fuse p orbital parts on both side of node plane as double bonds delocalised at joined groups of atoms, for example, >C=C-C=C-C=C< common for six carbon atoms which each has energy from -100 to -150 kJ/mol.

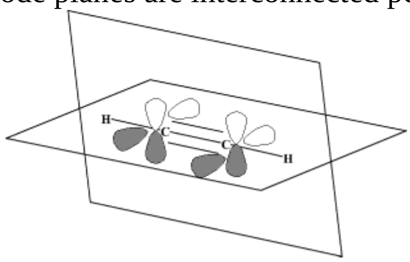
σ molecular orbital electron negative charge density increases on line, what connect atomic nuclei. π bond forms negative charge density increase between atoms (**C** and **C** or **O** or **S** or **P** or **N**) both side node planes. *Latin* word *singulāris – one, alone* in English and *Greeks* letter sigma σ is first letter of word and designate simple covalent bond – sigma bond. Double bond is paired bond >**C=C**< and *Latin* word *pār* –pair in English which first letter from *Greeks* alphabet is pi π which designate double or triple bond pi.

π orbital parallel to σ orbital - sigma covalent bond in ethane () in ethene  and ethyne (**H-C≡C-H**) as additional to σ bond (singular bond) are double and triple bonds. Naturally occurring π bond exist only in combination with σ bond as additional covalent bond into double and triple bonds.

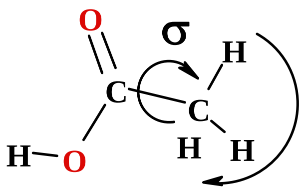
C=O ; **O=C=O** ; 

Carbon(II) oxide; carbon(IV) oxide; carbonic acid $\mathbf{H_2CO_3}$

Simple covalent bonds always are σ molecular orbitals, but double () and triple (**H-C≡C-H**) bonds are π molecular orbital (one or two) additional combination with simple covalent bond σ molecular orbital. Triple bond for both π orbitals node planes are interconnected perpendicular.

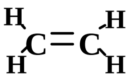


With σ bond connected atoms in molecule has rotation freedom dimension around symmetry axis of orbital.



Acetic acid molecule $\mathbf{HOOC\text{-}CH_3}$ between carbon atoms has sigma bond.

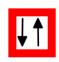
However double bond is solid, steady and consistent (*consistere* – *Latin* word – solid, firm, standing).

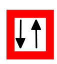
 ethene molecule is planar inflexible structure without rotation around >**C=C**< double bond.

Ethyne triple bond provides four atoms quite on linear structure **H-C≡C-H** straight stick form.

Exercise. Draw the structure formulas for given molecules! Account sigma σ and π bonds? Account and show π bonds between which atoms in molecule are formed? Oxygen $\mathbf{O_2}$, nitrogen $\mathbf{N_2}$, carbon(IV) oxide $\mathbf{CO_2}$, sulfur(IV) oxide $\mathbf{SO_2}$, sulfur(VI) oxide $\mathbf{SO_3}$, nitrogen(IV) oxide $\mathbf{NO_2}$, carbonic acid $\mathbf{H_2CO_3}$, sulfuric acid $\mathbf{H_2SO_4}$, phosphoric acid $\mathbf{H_3PO_4}$, acetic acid $\mathbf{CH_3COOH}$, acetone $\mathbf{CH_3COCH_3}$, calcium carbide $\mathbf{CaC_2}$, ethyne $\mathbf{C_2H_2}$.

Most important for covalent bond

1. Covalent bond between two atoms forms common electron pair in molecular orbital .

2. According exchange mechanism from each atom participate unpaired free electron  and  , forming common orbital with electron pair having opposite spins  .

3. Sigma σ bond is simple single covalent bond, which can get additional π bonds double or triple bonds.