Ķīmi 2028 PART II Organic compounds

Asoc.prof Anda Prikšāne anda.priksane@lu.lv

Requirements

- 4 Laboratory reports and tests
- 2 successfully passed tests
- Examination Part1 and part 2

```
* print out lab report in paper form, Exercise 1, 2,3

1st seminar: Test.

2nd Test: 4th of December
```

Textbooks

• Fundamentals of general, organic, and biological chemistry / J. McMurry., 7th ed. Pearson Education, 2013. p. 970 (e-book)

http://www.biblioteka.lu.lv/e-resursi/nozaru-e-gramatas/kimija/

• Foundations of organic chemistry: unity and diversity of structures, pathways, and reactions / by David R. Dalton., Wiley, [2011], p.1414. (e-book. *large*)

Textbooks

- 3. Groundwater P.W., TaylorG.A. Organic Chemistry, 1998, Longman.
- 4. Brown W., Foote C., Organic Chemistry, , Harcoutr College Publishers, 2002.
- 5. Organic Chemistry (Mc.Murry, Solomons T.W.G., Bruice etc.)
- 6. Organic chemistry: a brief course / David J. Hart .[u.c.]., 13th. ed., Brooks/Cole Cengage Learning, 2012., p.580.

Organic compounds

Organic chemistry is chemistry of carbon compounds.

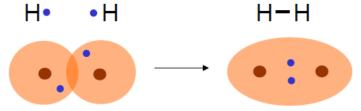
Carbon atoms are linked together or linked with H, O, Hal, N and also P.

Chemical bonds in organic compounds

- Carbon typically *engages in a total of four bonds* in a compound. These bonds can be distributed in several ways, *four* single bonds, one double bond and two single bonds, two double bonds or one triple bond and one single bond.
- Only valence electrons are used in chemical bonding in organic molecules.

The two extreme cases of chemical bonds

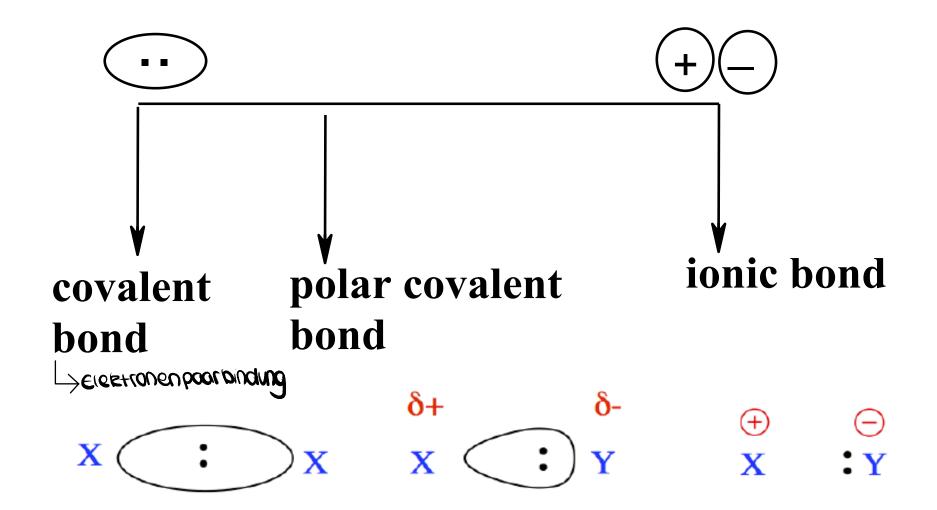
Covalent bond - in which one or more pairs of electrons are shared by two atoms.



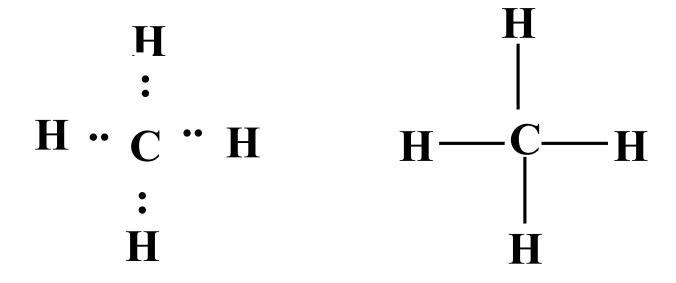
Ionic bond - bond in which one or more electrons from one atom are removed and attached to another atom, resulting in positive and negative ions which attract each other.

Na*: ci: \longrightarrow Na*: ci: \longrightarrow

Principles of bond formation



Covalent bonds of methane



Polar covalent bonds

Covalent bonds in which the sharing of the electron pair is unequal, are called polar covalent bonds.

$$_{3}^{\delta+}$$
 $_{3}^{\delta-}$ $_{3}^{\delta-}$ $_{3}^{\delta-}$ $_{3}^{\delta-}$ $_{3}^{\delta-}$ $_{3}^{\delta-}$ $_{4}^{\delta-}$ $_{5}^{\delta-}$ $_{5}$

In such a bond there is a charge separation with one atom being slightly more positive and the other more negative.

The ability of an atom to attract electrons in the presence of another atom is a measurable property called *electronegativity*:

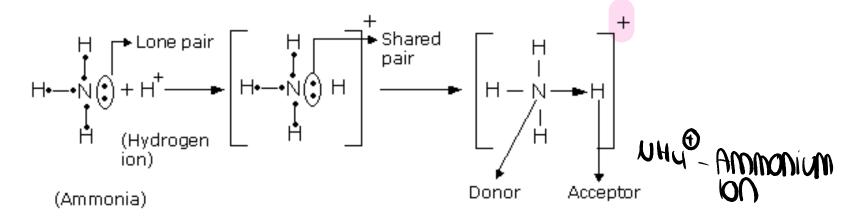
$$H - 2,1, C - 2,5, N - 3,0, Cl - 3,0.$$

Donor- acceptor bond

• The donor-acceptor bond is formed by a pair of electrons from one atom (the donor) and a free (unfilled) orbital from another (the acceptor). The difference can be expressed schematically:

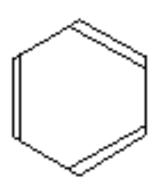
Covalent bond A + B->A:B

Donor-acceptor bond A: + B->A:B



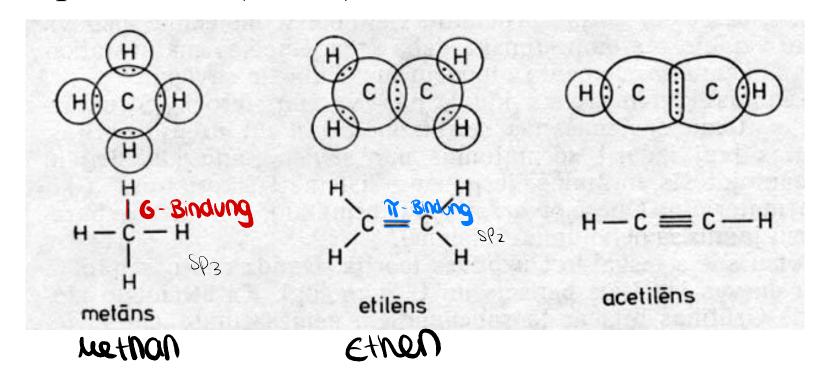
?

$H-C \equiv C-H$

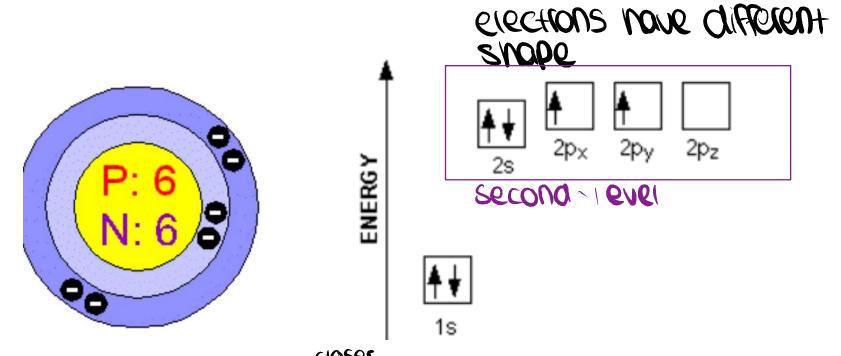


Types of covalent bonds

- single bond, (σ)
- double bonds, (σ, π)
- triple bonds $(\sigma \pi, \pi)$



Carbon atom



Number of Energy Levels: 2/ to the nucleus

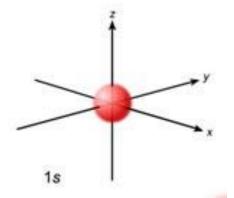
First Energy Level: 2 s electrons

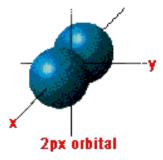
Second Energy Level: 2s electrons and 4 p valence electrons.

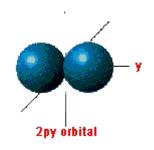
Electrons of s and p orbitals have different «shape».

s and p orbitals

- An orbital is a region of space in which there is a 99% probability of finding an electron with a specific quantity of energy.
- The 's' orbital is spherical about the nucleus and the 'p' orbitals are like double headed balloons arranged along the axis of (imaginary) three dimensional coordinates.



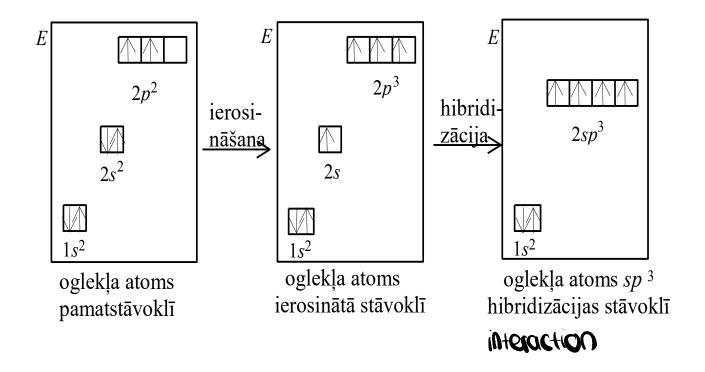




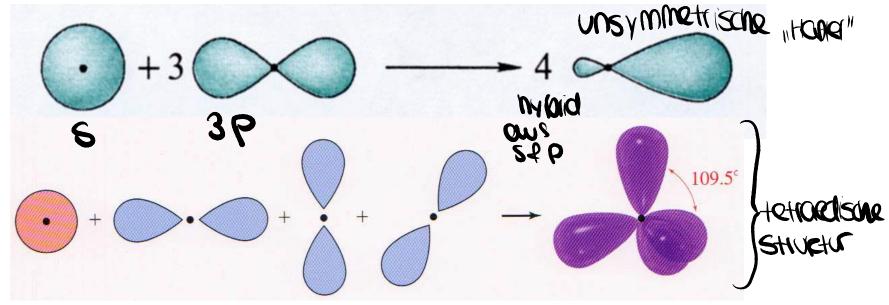
Valence electrons of carbon

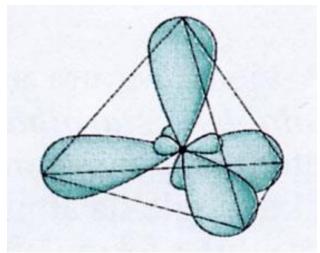
1.sp3 hybridisation

'p' orbitals



sp3 hybridisation



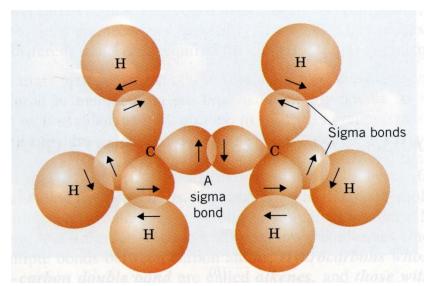


Methane Ethane

Alkanes in allen

Angle 109,28

Alkanes - Ethane



2 C atoms sp3,

 7σ bonds C-C, C-H

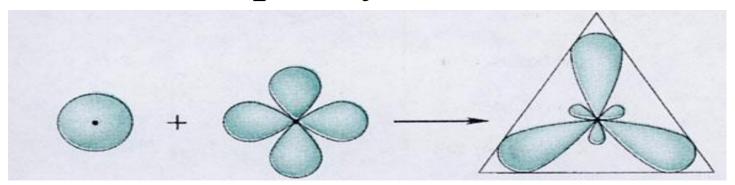
Propane 3 C atomi sp3, 10 σ bonds

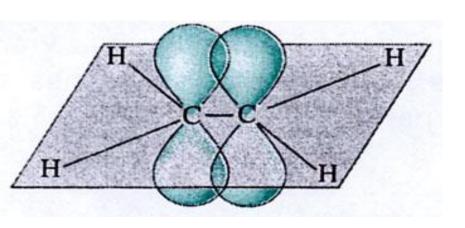


Reaction of substitution



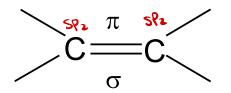
sp2 hybridisation





$$C=C$$

Ethene (alkene) 5σ bonds are in one plane, angles 120° π –bond is in the perpendicular plane

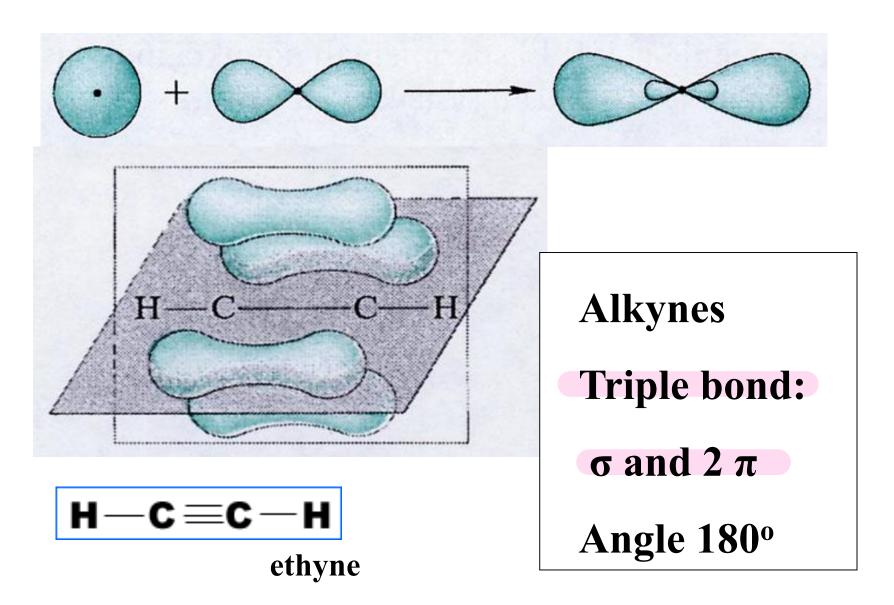


2C atoms are in Sp2 un 1C atom in sp3 hybridisation 8 σ bonds (C-C, C-H) and 1 π bond

Reaction of addition to double bond

Addition 1

sp hybridisation



2. Writing Structures

Molecular formulas

C6H12O6 glucose

• Structure formulas - *Line structures* are used for both linear and cyclic structures. In these structures it is understood that there is a carbon atom at each "bend" and that each carbon atom is attached to as many hydrogen atoms as are needed to complete its valence of four.

$$H = \begin{pmatrix} H & H & H \\ & & & \\ &$$

2.1.Isomers

Isomers - two or more compounds that have the same formula but different structures.

Structure isomers and stereoisomers

Moleculformula C₂H₆O

3. Reactions of organic compounds

Reaction of nucleophilic substitution S_N

Reagent - chlorine anion
$$Cl^-$$

$$C_3H_7-OH + HCl \longrightarrow Cl^- C-OH$$
substrate reagent (starting material)
$$C_3H_7-Cl + H_2O$$
product by-product transition state

Classification of organic reactions is based on reaction mechanisms.

3.1.Classification of organic reaction based on the type of reagent

- radical reactions,
- ionic reactions-
- electrophilic reactions,
- nucleophilic reactions

$$A : B \longrightarrow A^{+} + B$$
 homolytic fission \longrightarrow radicals

 $A : B \longrightarrow A^{+} + B$ heterolytic fission \longrightarrow ions

4.2. Examples of bond breaking

Radical reaction

$$\operatorname{Br} \cdot + \operatorname{H} \cdot \int_{\operatorname{CH}_{3}}^{\operatorname{H}} \operatorname{CH}_{3} \longrightarrow \operatorname{HBr} + \operatorname{CH}_{3} \cdot \operatorname{CH} - \operatorname{CH}_{3}$$

Ionic reaction

$$C_3H_7$$
 - Br + OH - \longrightarrow C_3H_7 - OH + Br -





Radicals

Cl·, Br·, ·O - O·

Ions and neutral molecules



Nuclophils

OH⁻, RO⁻, RCOO⁻, Hal⁻, NH₃, H₂Ö

Electrophils

H⁺, H₃O⁺, NO₂⁺, SO₃H⁺, Alk⁺, RCO⁺, AlCl₃, ZnCl₂

4.3. Main types of organic reactions

> substition

$$CH_4 + Br_2 \rightarrow CH_3 Br + HBr$$

addition (to double of triple bond)

$$CH_2 = CH - CH_2 - CH_3 + Cl_2 \longrightarrow CH_2 - CH - CH_2 - CH_3$$

$$Cl \quad Cl$$

$$1,2-dichlorobutane$$

> elimination (um reaction)

$$CH_3 \xrightarrow{H_2SO_4} CH_3 \xrightarrow{H_2SO_4} CH_3 - CH = CH_2 + H_2O$$

> oxydation (O2, KMnO4, etc.)

$$3CH_2 = CH_2 + 2KMnO_4 + 4H_2O \rightarrow 3CH_2 - CH_2 + 2KOH + 2MnO_2$$

OH OH

reduction (H2, NaBH4, LiAlH4)

$$CH_3^{+2} CH_3 \xrightarrow{[H]} CH_3^{-1} CH_3 CH_3$$

$$O OH$$

> condensation

 $[H] = H_2 \quad NaBH_4 \quad LiAIH_4$

 $[O] = O_2 \quad KMnO_4 \quad K_2Cr_2O_7$

Thank you!

Single: SO3

double + Single: SP2

$$+ \text{riple} + \text{single} = \text{sp}$$
 $+ \text{riple} + \text{single} = \text{sp}$
 $+ \text{riple} + \text{single} = \text{single} = \text{sp}$
 $+ \text{riple} + \text{single} = \text{single} = \text{single} = \text{single}$