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Introduction to organic chemistry

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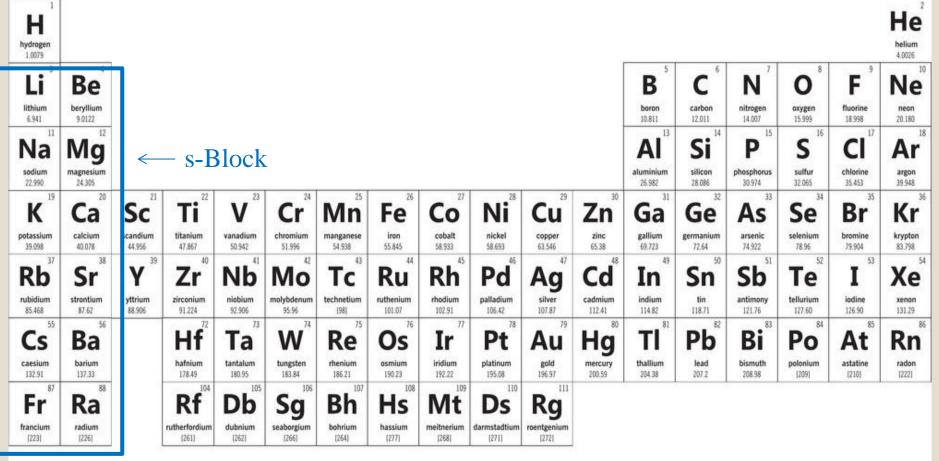
Krasnoyarsk, 2021

The subjects of organic chemistry are carbon-based (has the C–H bond)

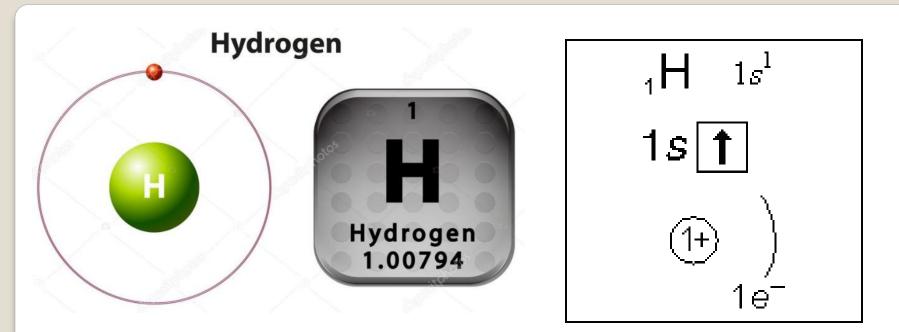
What is studied in organic chemistry? Can we build a wall between organic and inorganic chemistry?

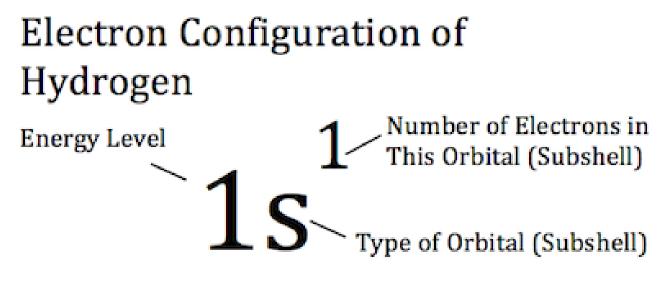
- Chemical elements that are necessary for the construction and life of cells and organisms are called biogenic elements. All living systems are based on six elements: carbon C, hydrogen H, oxygen O, nitrogen N, phosphorus P, and sulfur S, which are called <u>organogens</u> (97% of them).
- In addition, vital macroelements also include s-elements of the third (sodium, magnesium) and fourth (potassium, calcium) periods, and p-elements of the third period (chlorine).

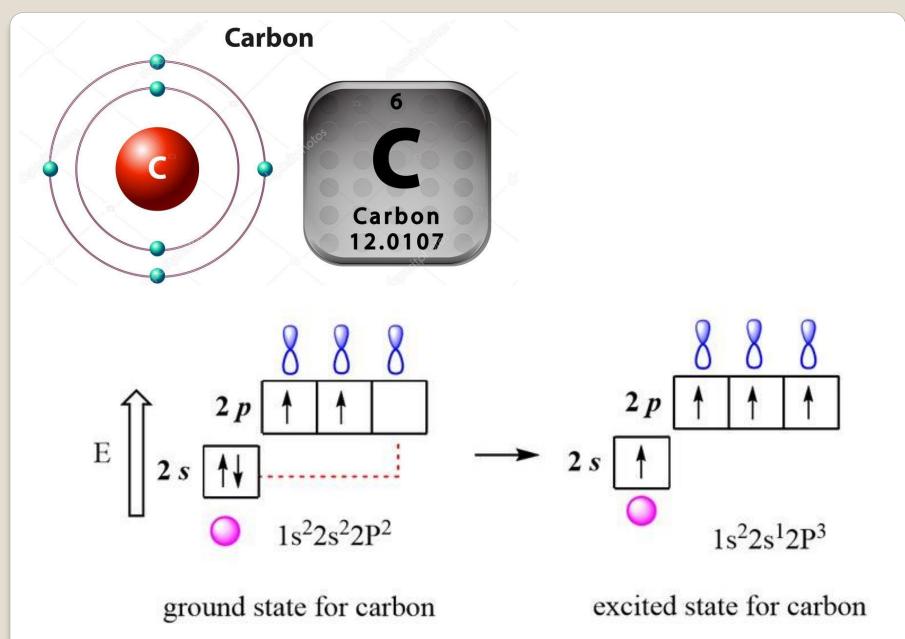
Periodic Table of the Elements

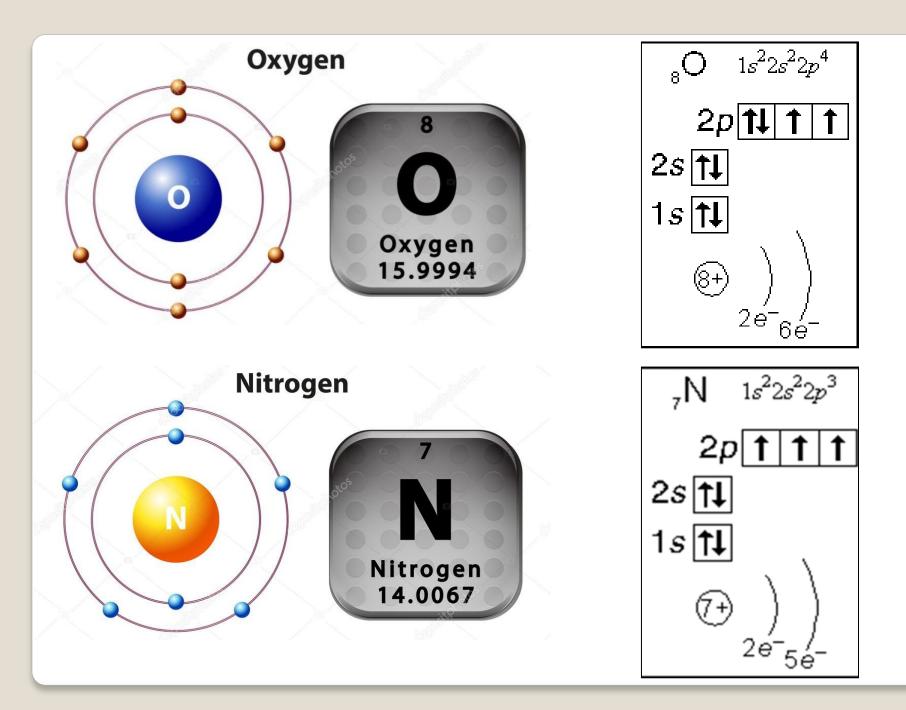


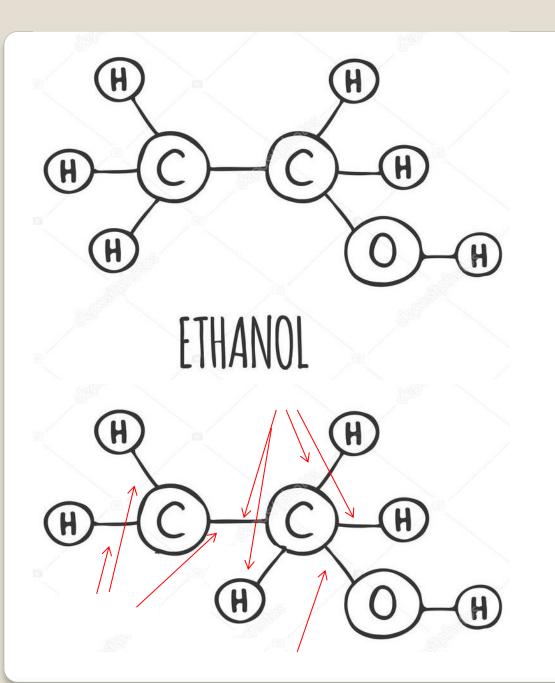
La ⁵⁷	Ce ^{ss}	Pr	Nd	Pm	Sm	Eu	Gd	Τb	Dy	Ho	Er	Tm	Yb	Lu
lanthanum	cerium	praseodymium	neodymium	promethium	samarium	europium	gadolinium	terbium	dysprosium	holmium	erbium	thulium	ytterbium	lutetium
138.91	140.12	140.91	144.24	[145]	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.05	174.97
Ac	Th	Pa	U ⁹²	Np	Pu	Am	Cm	Bk	Cf [®]	Es	Fm	Md	No	Lr
actinium	thorium	protactinium	uranium	neptunium	plutonium	americium	curium	berkelium	californium	einsteinium	fermium	mendelevium	nobelium	lawrencium
[227]	232.04	231.04	238.03	[237]	(244)	(243)	[247]	[247]	[251]	[252]	(257)	[258]	(259)	[262]



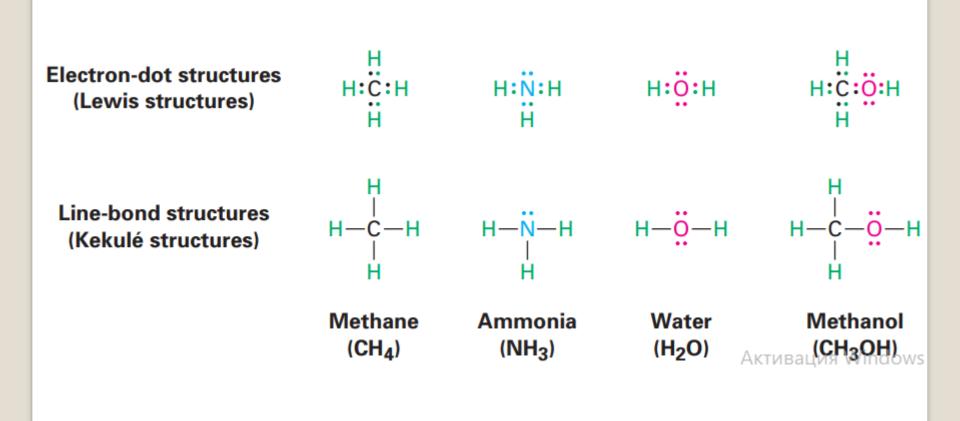








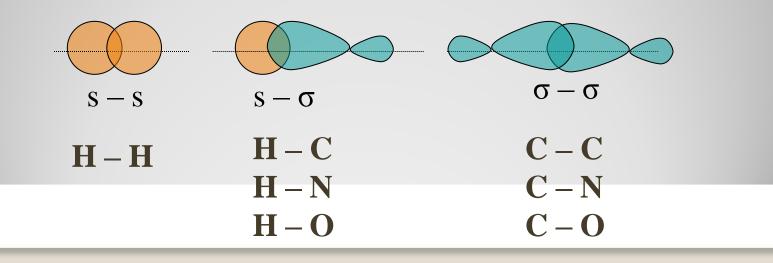




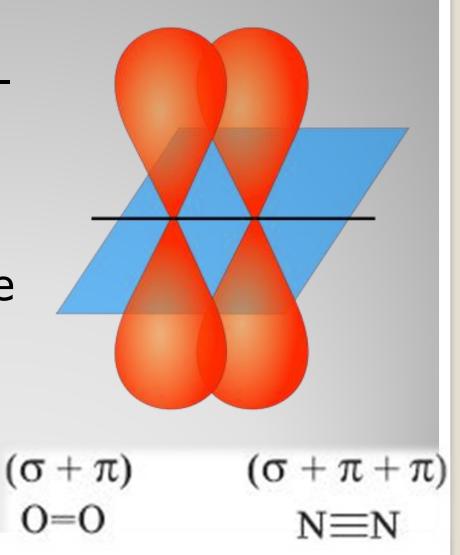
- Bond multiplicity is the number of electron pairs socialized by neighboring atoms as a result of the formation of a covalent bond.
- In ethane, H₃C-CH₃ bond between carbon atoms is single, in ethylene, H₂C=CH₂ double, in acetylene, HC=CH - triple.

(
$$\sigma$$
) ($\sigma + \pi$) ($\sigma + \pi + \pi$)
F—F 0=0 N \equiv N

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.



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

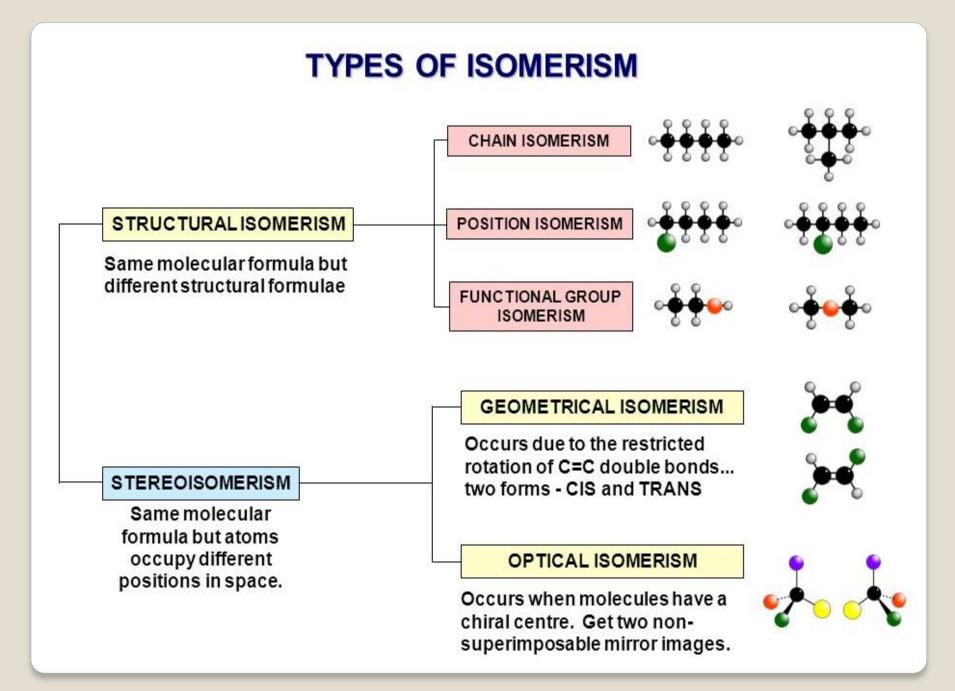


Isomerism

Isomers are molecules with identical molecular formulae that is, same number of atoms of each element — but distinct arrangements of atoms in space. Isomerism is existence or possibility of isomers.

Use handouts.

 Read the text "Isomerism" WB1, p. 15; WB2 p. 15. How many types of this phenomenon can be distinguished?



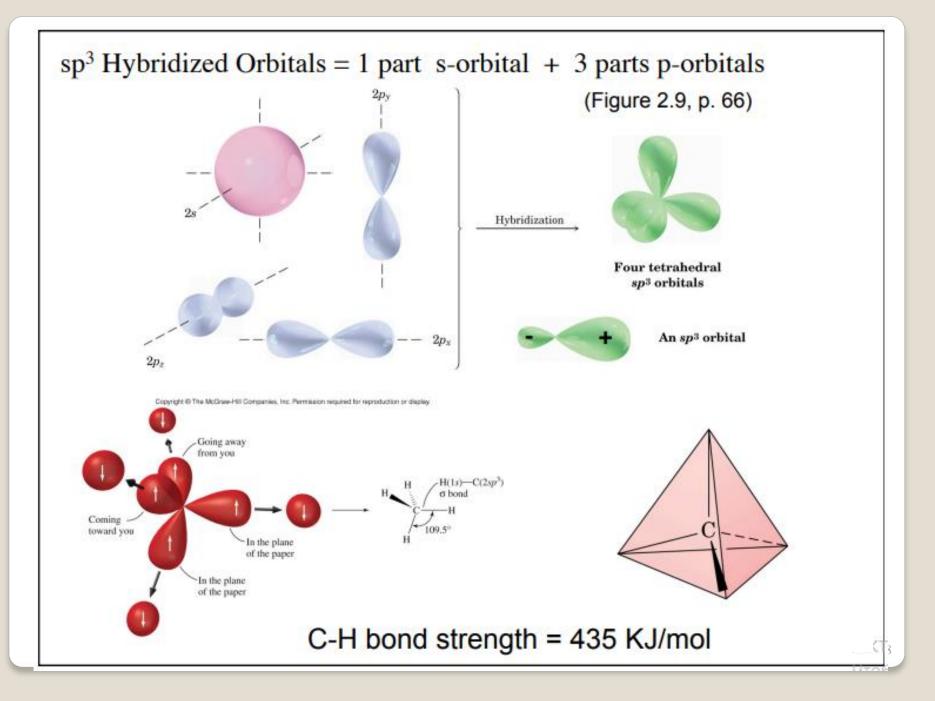
Use handouts.

- Read the text "Isomerism". How many types of this phenomenon can be distinguished?
- Do task 1 (practice) WB1, p. 15
- Read the text "Optical isomerism" WB2 p. 15
- Do task 1, 2, 3, 4 (a, b) WB2 p.
 15(!mark)

Hybridization

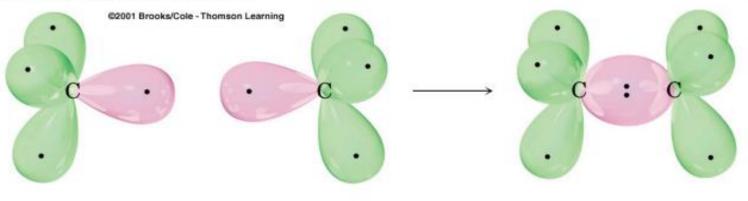
- HYBRIDIZATION is the mixing of atomic orbitals of different shapes and energies (within the valence level) with the formation of atomic orbitals of the same shape and energy.
- When s-AO and p-AO are mixed, hybrid atomic orbitals (σ AO) are formed:

$$s - AO \qquad p - AO \qquad \sigma - AO \\ (hybrid) \\ (!video)$$



sp³ hybridized orbital are more directional allowing for greater orbital overlap and strong bonds compared to unhybridized orbitals

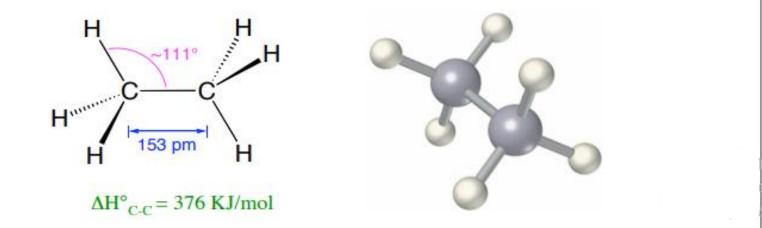
2.7: Bonding in Ethane

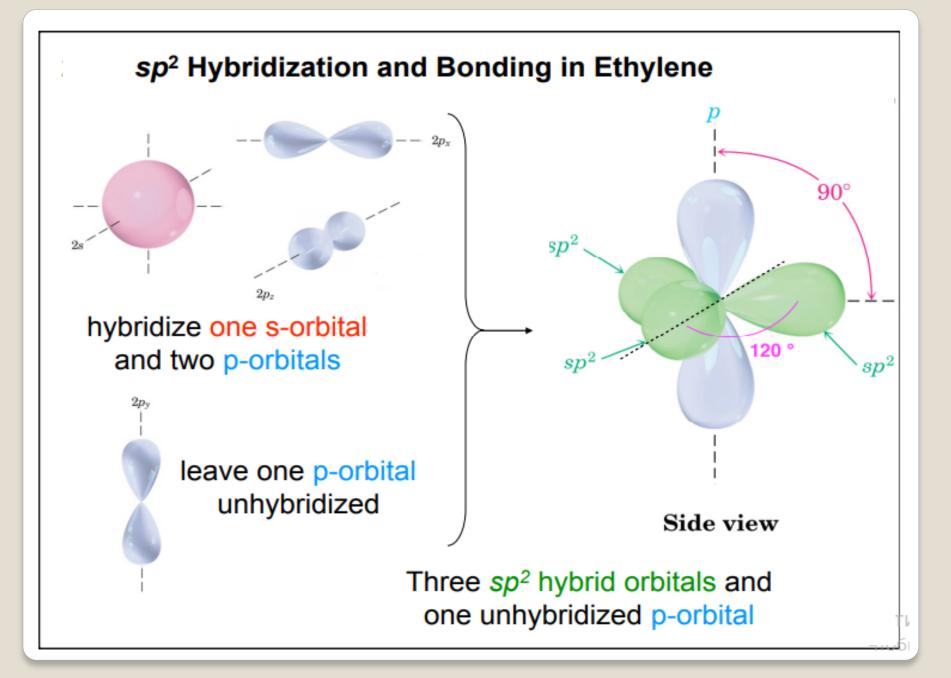


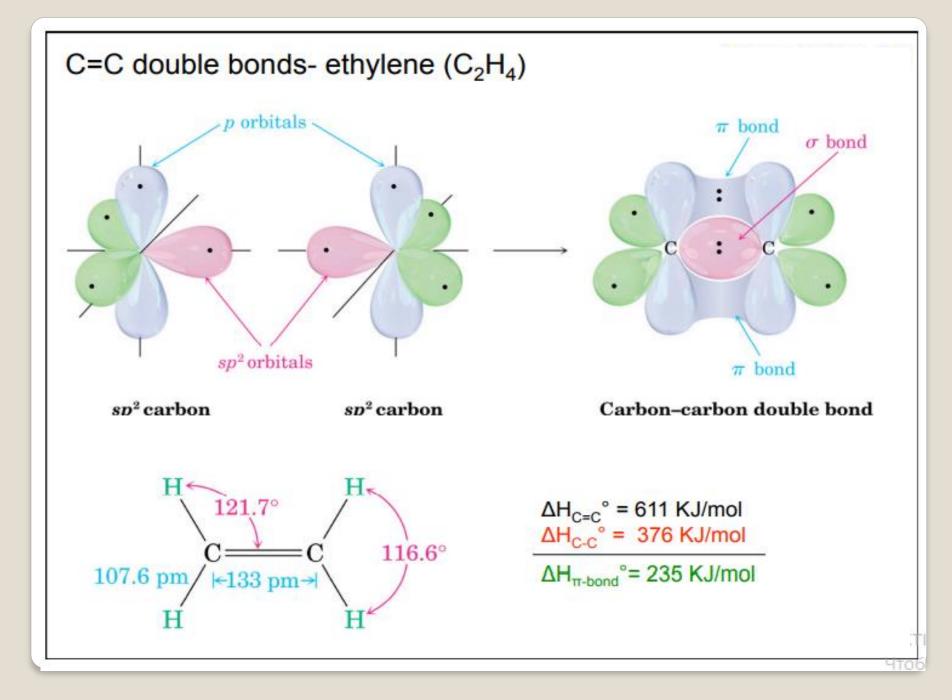
 $sp^3-sp^3\sigma bond$

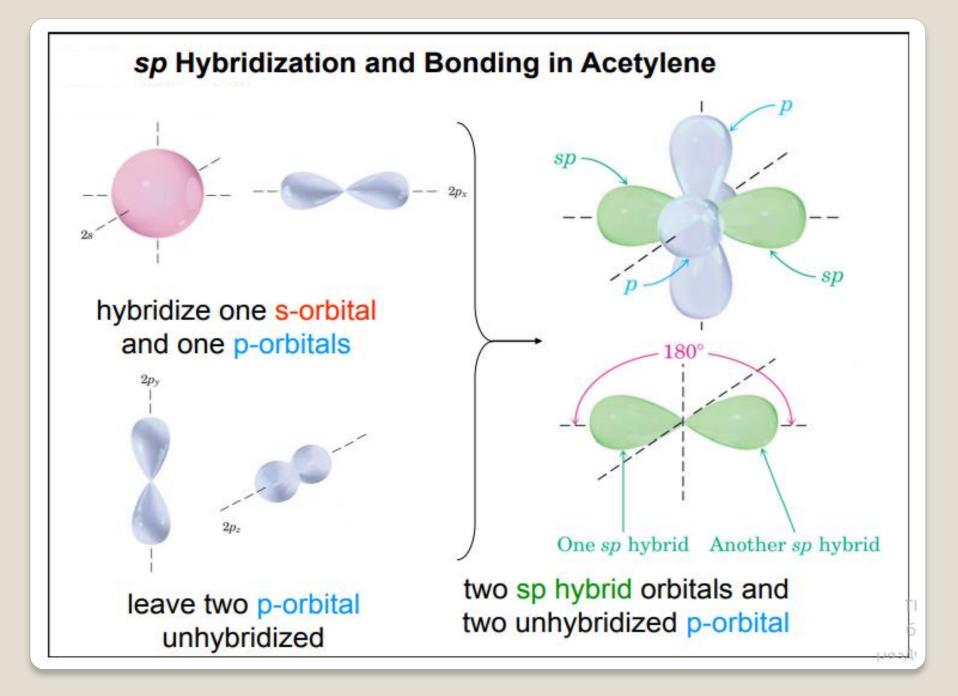
sp³ carbon

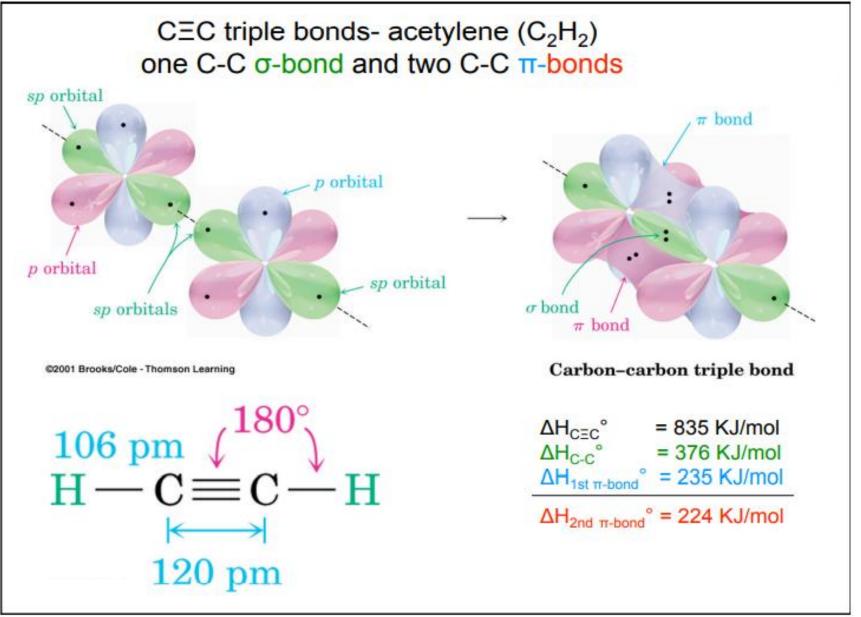
sp³ carbon











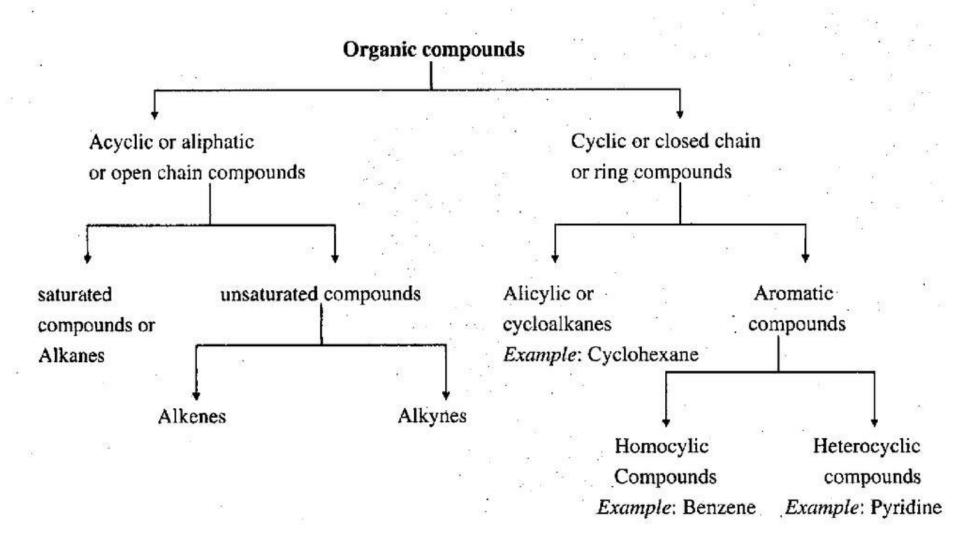
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Type of Hybridiza tion	Formula	Carbon skeleton structure	view				
sp	1s + 1p = 2sp	linear (180°) C					
sp ²	1s + 2p = 3sp ²	flat triangle (120°) ==C					
sp ³	1s + 3p = 4sp ³	tetrahedral (109°)					
TYPES OF HYBRIDIZATION OF ATOMIC ORBITALS							

Determine the hybridization of each carbon atom in the following molecules: (a) H_3C-CH_3 (!mark) (b) $H_3C-CH=CH_2$ (c) $CH_3-C\equiv C-CH_2OH$ (d) $CH_3CH=O$ (e) CH_3COOH

Classification of organic compounds

Schematic representation for the classification of organic compounds



Class	General Formula	Example	Common Name (Systematic Name)	Common Suffix/Prefix (Systematic)	
		Hydrocarbons (УГЛ	ЕВОДОРОДЫ)		
Alkanes (Алканы)	RH	CH ₃ CH ₃	ethane (этан)	-ane (-ан)	
Alkenes (Алкены)	RR'C=CR"R"	H ₂ C=CH ₂	ethylene (этилен) (ethene) _(этен)	-ene (- <u>ен</u>)	
Alkynes (Алкины)	RC≡CR'	HC=CH	acetylene(ацетилен) (ethyne) _{(этин})	(-yne) (-ин)	
Arenes (Арены)	ArH°		benzene (бензол)	-ene (-бензол)	
	Ox	ygen-Containing Compou	nds(КИСЛОРОДСОДЕРЖА	АЩИЕ СОЕДИНЕНИ	
Alcohols (Спирты)	ROH [°]	CH ₃ CH ₂ OH	ethyl alcohol (ethanol) (этанол)	-оі (-од)	
Phenols (Фенолы)	$ArOH^{\flat}$	ОН	phenol (фенол)	-оl (- <u>ол</u>)	
Ethers (Простые эфиры)	ROR'	H ₃ CH ₂ COCH ₂ CH ₃	diethyl ether (диэтиловый	į́ether(-эфир)	
Aldehydes (Альдегиды)	RCHO	О Ц СН ₃ СН	эфир) acetaldehyde (ethanal) (<u>этаналь</u>)	-aldehyde (-al) (-аль)	
Ketones (Кетоны)	RR′C≡O	CH ₃ CCH ₃	acetone (2-propanone)(<u>пропанон</u>)	-one (-он)	
Carboxylic acids (Карбоновые кислоты)	RCO ₂ H	о СН ₃ СОН	acetic acid (ethanoic acid)(<u>этановая</u>	-ic acid (- <u>овая</u> (-oic acid) _{кислота}	
(Nit	rogen-Containing Compo	unds (АЗОТСОДЕРЖАЩЍЕ	соединения)	
Amines (Амины)	RNH ₂ , RNHR', RNR'R"	CH ₃ CH ₂ NH ₂	ethylamine (<u>этиламин</u>)	-amine (-амин)	
Nitriles (Нитрилы)	RC≡N	$H_3CC \equiv N$	acetonitrile (ацетонитрил	<u>י)</u> -nitrile (-нитрил)	
Nitro compounds (Нитро соединения)	ArNO ₂ °		nitrobenzene(нитробензо	л)nitro- (нитро <u>-)</u>	

TABLE 11.9 Classific	cation of Organic Compour	nas	
Class	Example	Functional Group	Characteristic
Alkene	$H_2C = CH_2$	∑c=c<	Carbon-carbon double bond
Alkyne	НС≡СН	$-c \equiv c -$	Carbon-carbon triple bond
Aromatic	H H H H H H H H H H	\bigcirc	Benzene ring (six carbon atoms and six hydrogen atoms)
Haloalkane	CH ₃ —Cl	F,	One or more halogen atoms
Alcohol	CH ₃ —CH ₂ —OH	—ОН	Hydroxyl group (—OH)
Ether	CH ₃ —O—CH ₃	—o—	Oxygen atom bonded to two carbons
Thiol	CH ₃ —SH	—SH	Thiol group (-SH)
Aldehyde	$CH_3 - C - H$	о ∥ —С—н	Carbonyl group (carbon–oxygen double bond) with —H
Ketone	CH ₃ —CH ₃		Carbonyl group (carbon–oxygen double bond) between carbon atoms
Carboxylic acid	$CH_3 - C - O - H$	о —С—О—Н	Carboxyl group (carbon–oxygen double bond and —OH)
Ester	СН ₃ —С—О—СН ₃		Carboxyl group with -H replaced by a carbon
Amine	CH3-NH2	— <u>N</u> —	Nitrogen atom with one or more carbon groups
Amide	$\mathbf{CH}_{3} - \mathbf{C} - \mathbf{NH}_{2}$	-C - N -	Carbonyl group bonded to nitrogen

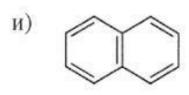
TABLE 11.9 Classification of Organic Compounds

	Structures of Some	Common Functional G	iroups				
Name	Structure*	Name ending	Example	Name	Structure*	Name ending	Example
Alkene (double bond)	}c=c	-ene	H ₂ C—CH ₂ Ethene	Sulfide	\sim^{s}	sulfide	CH ₃ SCH ₃ Dimethyl sulfide
Alkyne (triple bond)	-C-C-	-yme	HC==CH Ethyne	Disulfide	X	disulfide	CH ₃ SSCH ₃ Dimethyl disulfide
Arene (aromatic ring)	\rightarrow	None	Benzene	Carbonyl	۰۰ ۲ بر		
Halide	(X = F, Cl, Br, I)	None	CH ₃ CI Chloromethane	Aldehyde	,e ,	-al	CH ₃ CH Ethanal
Alcohol	X OH	-ol	CH ₃ OH Methanol	Ketone		-one	CH3CCH3
Ether	$\sim \sim$	ether	CH ₃ OCH ₃ Dimethyl ether	Contractionsia	ΛΛ	-oic acid	Propanone
Monophosphate		phosphate	CH30P03 ²⁻ Methyl phosphate	Carboxylic acid	С С ОН	-oic acia	CH ₃ COH Ethanoic acid
Amine	X	-amine	CH ₃ NH ₂ Methylamine	Ester	X	-oate	CH ₃ COCH ₃ Methyl ethanoate
Imine (Schiff base)		None	NH CH ₃ CCH ₃ Acetone imine	Amide	N. N	-amide	CH ₃ CNH ₂ Ethanamide
Nitrile	-C=N	-nitrile	CH ₃ C=N Ethanenitrile	Carboxylic acid anhydride	1	-oic anhydride	сн _з соссн _з
Nitro	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	None	CH ₃ NO ₂ Nitromethane	-	Xox	and addressed a	Ethanoic anhydride
Thiol	X SH	-thiol	CH ₃ SH Methanethiol	Carboxylic acid chloride	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	-oyl chloride	O II CH3CCI Ethanoyl chloride

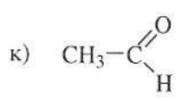
Determine the class and C-chain type of organic compounds

- CH₃-CH₂-C a)
- CH₃-CH₂-Br б)
- CH₃-CH₂-OH B)
- CH₃-CH=CH-CH₃ **Г**)
- $CH_3 C \equiv C CH_3$ $CH_3 CH_2 NH_2$ Д)
- e)

CH₃-CH₂-O-CH₂-CH₃ ж) 3) CH₃-C-CH₃



(!mark)



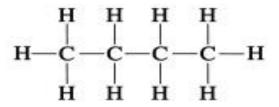
Nomenclature of organic compounds

Summary of Formulas

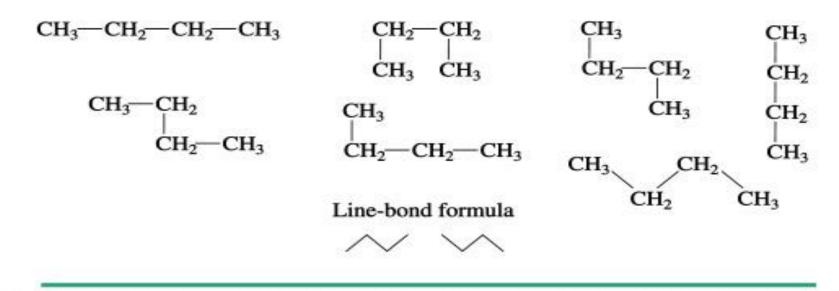
Table 12.3 Some Structural Formulas and Conformations for Butane C₄H₁₀

Expanded structural formula

Molecular formula



Condensed structural formulas



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IUPAC System of Naming Alkanes

- The **IUPAC** (International Union of Pure and Applied Chemistry) establishes the rules for naming organic compounds.
- Alkanes are named with –ane endings.
- The first four alkanes are methane, ethane, propane and butane.
- The names of longer carbon chains use Greek prefixes such as *pent*- for 5 C atoms and *hex*- for 6 C atoms.

Table 12.1 IUPAC Names for the First Ten Continuous-Chain Alkanes

Number

Prefix	Name	Molecular Formula	Condensed Structural Formula
Meth	Methane	CH4	CH4
Eth	Ethane	C ₂ H ₆	CH ₃ CH ₃
Prop	Propane	C ₃ H ₈	CH ₃ CH ₂ CH ₃
But	Butane	C4H10	CH ₃ -CH ₂ -CH ₂ -CH ₃
Pent	Pentane	C5H12	CH ₃ CH ₂ CH ₂ CH ₂ CH ₃
Hex	Hexane	C ₆ H ₁₄	CH ₃ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃
Hept	Heptane		CH ₃ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃
Oct	Octane	C8H18	CH ₃ -CH ₂ -CH ₃
Non	Nonane	C ₉ H ₂₀	CH ₃ -CH ₂ -CH ₃
Dec	Decane	C10H22	CH ₃ CH ₂ CH
	Meth Eth Prop But Pent Hex Hept Oct Non	MethMethaneEthEthanePropPropaneButButanePentPentaneHexHexaneHeptHeptaneOctOctaneNonNonane	PrefixNameFormulaMethMethane CH_4 EthEthane C_2H_6 PropPropane C_3H_8 ButButane C_4H_{10} PentPentane C_5H_{12} HexHexane C_6H_{14} HeptHeptane C_7H_{16} OctOctane C_8H_{18} NonNonane C_9H_{20}

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Learning Check

- A. Give the name of each compound:
 1) CH₃-CH₃
 2) CH₃-CH₂-CH₃
 3) CH₃-CH₂-CH₂-CH₂-CH₂-CH₂-CH₂-CH₃
- B. Write the condensed structural formula of pentane.

Solution

A. Give the name of each compound: 1) CH₃-CH₃ ethane 2) CH₃-CH₂-CH₃ propane 3) CH₃-CH₂-CH₂-CH₂-CH₂-CH₂-CH₂-CH₃ hexane

B. Write the condensed structural formula of pentane. CH₃-CH₂-CH₂-CH₂-CH₂-CH₃

Learning Check

For propane, write the:

- 1) Molecular formula
- 2) Expanded structural formula
- 3) Condensed structural formula (two conformations)
- 4) Line-bond formula

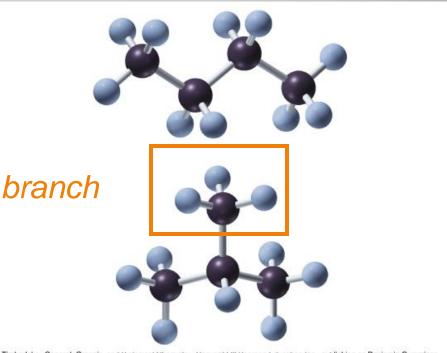
Solution

1) Molecular formula C_3H_8 2) Expanded structural formula ннн н – с– с– с– н 3) Condensed structural formula (two conformations) CH₃-CH₂-CH₃ **CH**₃ CH₃-CH₂

4) Line-bond formula

Branched-Chain Alkanes

 In a branchedchain alkane, a side group called a branch or a substituent is attached to a carbon chain.



Alkyl Groups

An alkyl group:

- Is composed of one or more carbon atoms attached to a carbon chain.
- Is derived from the corresponding alkane by removing one hydrogen.
- Is named by replacing the –ane ending of the corresponding alkane with –yl.
- Derived from methane is *methyl* and from ethane is *ethyl*.

Name of Alkane	Corresponding Alkyl Group	Name of Alkyl Group
Methane	СН ₃ —	Methyl
Ethane	CH ₃ -CH ₂ -	Ethyl
Propane	CH ₃ -CH ₂ -CH ₂ -	Propyl
	СН3-СН-СН3	Isopropyl
Butane	CH3-CH2-CH2-CH2-	Butyl
	CH ₃ —CH—CH ₂ —CH ₃	sec-Butyl
	CH.	(secondary butyl)
The Local Date of the		L . L . I
Isobutane		Isobutyl
	CH ₃	
	CH ₃ -C-CH ₃	tert-Butyl or t-butyl (tertiary butyl)
	Alkane Methane Ethane Propane	AlkaneAlkyl GroupMethane $CH_3 - $ Ethane $CH_3 - CH_2 - $ Propane $CH_3 - CH_2 - CH_2 - $ $H_3 - CH_3 - CH_3 - CH_3$ Butane $CH_3 - CH_2 - CH_2 - CH_2 - $ $CH_3 - CH_2 - CH_2 - CH_2 - $ $CH_3 - CH_2 - CH_2 - CH_3$ Isobutane $CH_3 - CH_3 - CH_2 - CH_2 - $ $CH_3 - CH_3 - CH_2 - CH_3 - $

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Naming Branched-Chain Alkanes

The names of branched-chain alkanes indicate the groups bonded to the longest carbon chain.

CH₃ methyl group on C-3

 $CH_3 - CH_2 - CH_2 - CH_2 - CH_2 - CH_3$ hexane 6 5 4 3 2 1

3-Methylhexane

Naming Summary

In the IUPAC system:

- The longest chain is named as the main chain.
- Any carbon branches use their alkyl names.
- Each branch is numbered by counting the main chain from the end nearest the first side group.
- Branches are listed in alphabetical order.

Learning Check

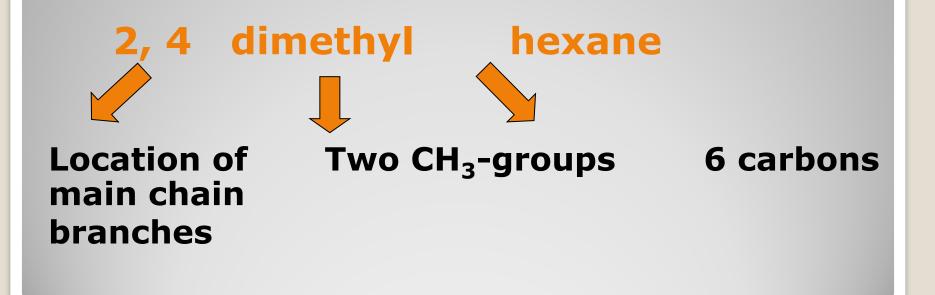
Give the IUPAC name for each alkane. CH₃ CH₃ Α. $CH_3 - CH - CH_2 - CH - CH_3$ Β. CH_2CH_3 CH_3 $CH_3 - CH_2 - CH_2 - CH_2 - CH_2 - CH_3$

Solution

CH₃ CH₃ Α. $CH_3 - CH - CH_2 - CH - CH_3$ 2,4-dimethylpentane Β. CH_2CH_3 CH_3 $CH_3 - CH_2 - CH - CH_2 - C - CH_2 - CH_3$ CH₃ 5-ethyl-3,3-dimethylheptane

What Is In A Name?

The structural formula is drawn from the IUPAC name. 2, 4-dimethylhexane



Drawing Structural Formulas

Draw the condensed formula of 2-methylpentane

- 1. Draw the main chain of 5 carbon atoms. C-C-C-C-C
- 2. Add a CH₃ branch to C-2 on the main chain. CH₃

c-c-c-c

3. Add hydrogen atoms to give 4 bonds to each C.
CH₃

$$CH_3 - CH - CH_2 - CH_2 - CH_3$$

Learning Check

Draw the condensed structural formula for

A. 2, 3-dimethylbutane

B. 2, 3, 4-trimethylpentane

Solution

Write the condensed structural formula for

- A. 2, 3-dimethylbutane CH₃ CH₃ I CH₃-CH-CH-CH₃
- B. 2, 3, 4-trimethylpentane CH_3 CH_3 CH_3 I I I $CH_3-CH-CH-CH-CH_{493}$

Other cases

How to give an IUPAC name for unsaturated hydrocarbons?
What if is there a functional group?

• Location!

Haloalkanes

- In a haloalkane, one or more H atoms in an alkane is replaced by a halogen atom.
- Haloalkanes containing one halogen are named alkyl halides.
- In IUPAC names, a halogen is named as fluoro, chloro, bromo, or iodo.
- CH₃Br bromomethane (methyl bromide)

```
CH_3 - CH - CH_2 - CH_3
```

2-chlorobutane (sec-butyl chloride)

Substituents

Two or more substituents are named in alphabetical order.
 CI Br
 I
 CH₃-CH-CH₂-CH-CH₂-CH₂-CH₃
 4-bromo-2-chlorohexane

Learning Check

The name of this compound is: CI CH₃ | | CH₃-CH₂-CH-CH₂-CH-CH₃

- 1) 2,4-dimethylhexane
- 2) 3-chloro-5-methylhexane
- 3) 4-chloro-2-methylhexane

Solution

The name of this compound is: CI CH₃ | | CH₃-CH₂-CH-CH₂-CH-CH₃

3) 4-chloro-2-methylhexane

Learning Check

Give the IUPAC name for each.

A. $CH_3CH_2 - F$ Br Cl | | B. $CH_3 - CH - CH - CH_3$

Solution

Give the IUPAC name for each. A. CH_3CH_2 -F fluoroethane

Br Cl | | B. CH₃-CH-CH-CH₃ <u>2-bromo-3-chlorobutane</u>

Learning Check

Halothane is widely used as an anesthetic, which is a compound that decreases the ability of the nerve cells to conduct pain.

What is the IUPAC name of halothane?

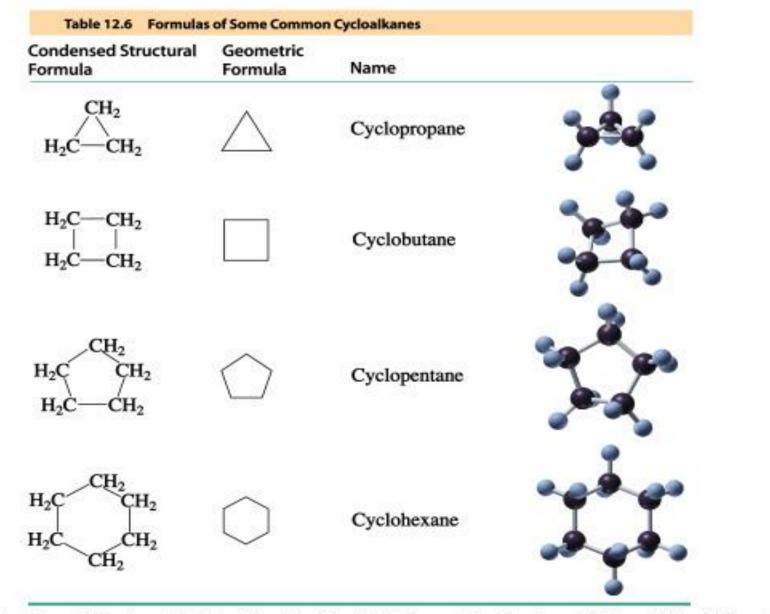
Solution

The IUPAC name is 2-bromo-2-chloro-1,1,1-trifluoroethane FBr III F-C-C-CI III FH

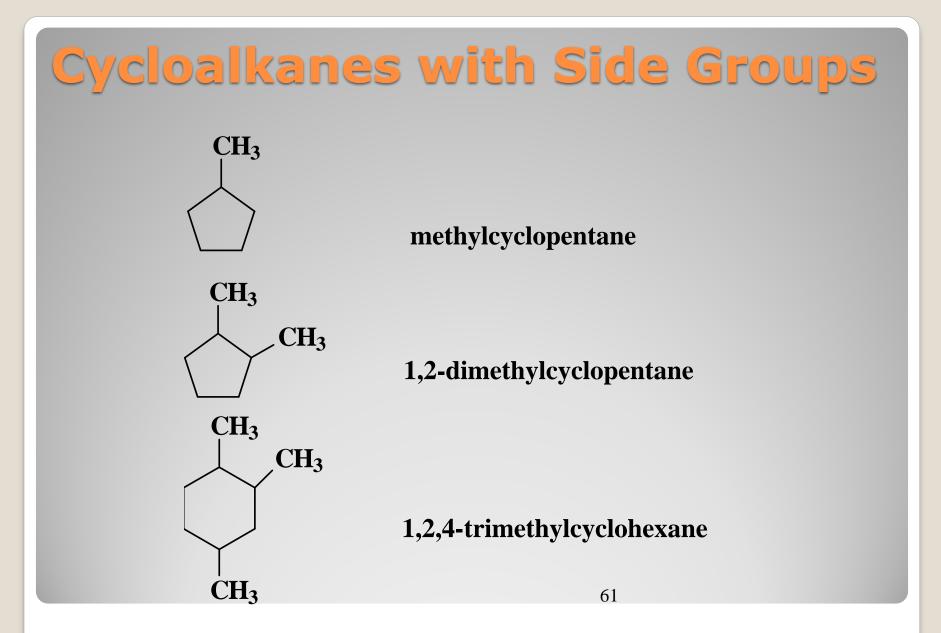
Other cases

How to give an IUPAC name for cyclic chain?

Cyclo!



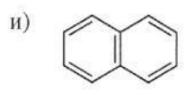
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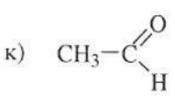
Give the IUPAC name

- a) CH₃-CH₂-C
- б) CH₃-CH₂-Br
- в) CH₃-CH₂-OH
- г) CH₃-CH=CH-CH₃
- $_{\text{д}})$ CH₃-C=C-CH₃
- e) CH₃-CH₂-NH₂

- ж) CH₃-CH₂-O-CH₂-CH₃
- 3) CH₃-C-CH₃

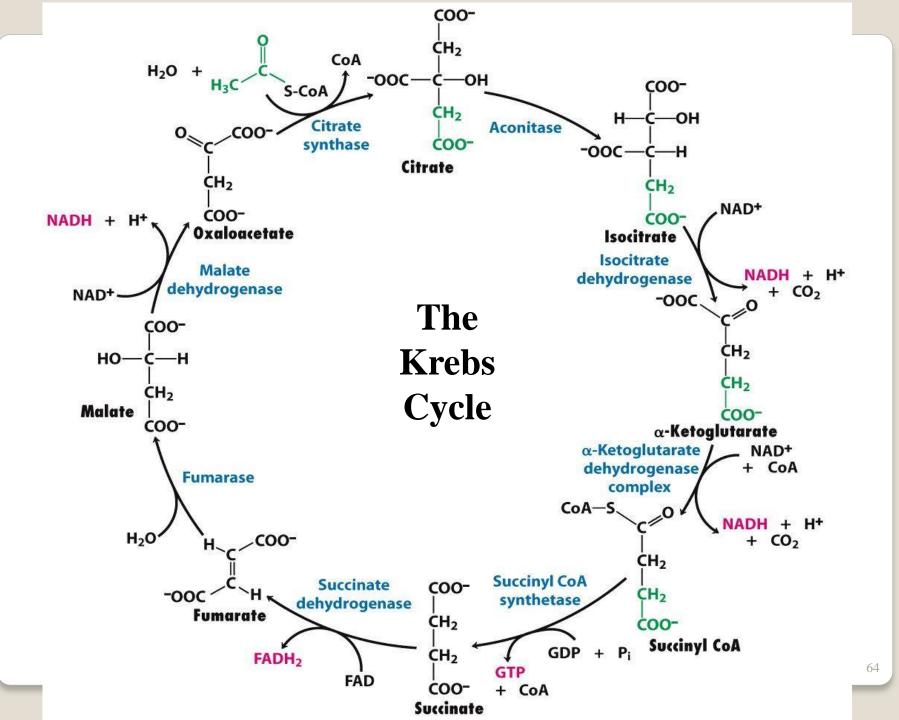


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HOMEWORK

<u>WB 1</u>. P.12, tasks 1, 2, 4, 5



HOMEWORK

1. Prepare for the test (Unit 1 Structure of organic compounds):

- Describe the electronic structure of organogenic atoms, their valence. Valence states of organogenic atoms. The types of hybridization. The main approaches to the classification of organic compounds.
- Isomerism of organic compounds.
- Nomenclature of Organic Compounds (IUPAC).
- Types of reagents, homolysis and heterolysis of covalent bonds, classification of organic reactions by direction and reagent involved. Types of reaction centers in molecules of organic compounds.

2. STUDY INFORMATION of the lecture "Alkenes and arenes reactivity"

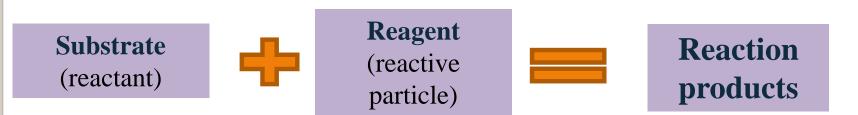
Types of reactions and reagents in organic chemistry

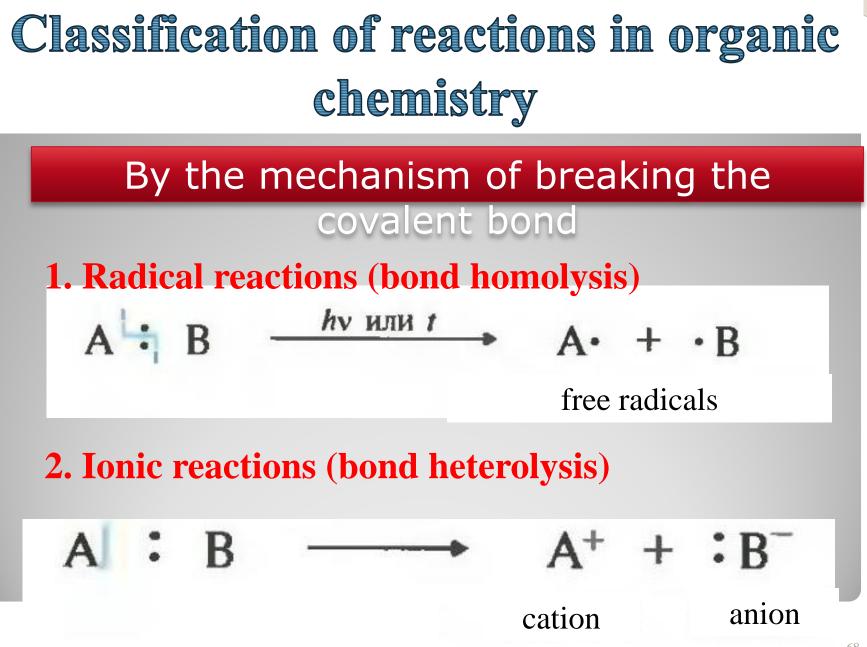
 A chemical reaction is a process accompanied by a change in the distribution of electrons in the outer shells of the atoms of the reacting substances.

Reactivity is the ability of a substance to react chemically and react at a slower or faster rate.

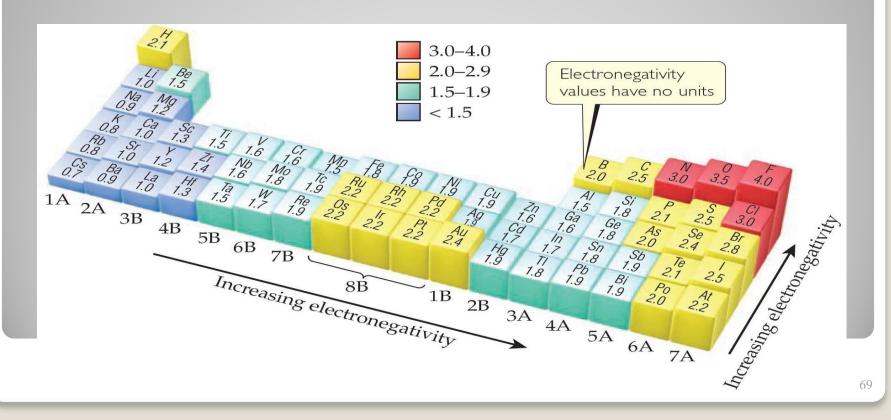
A reaction center is an atom or group of atoms directly involved in a given chemical reaction.







- 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.





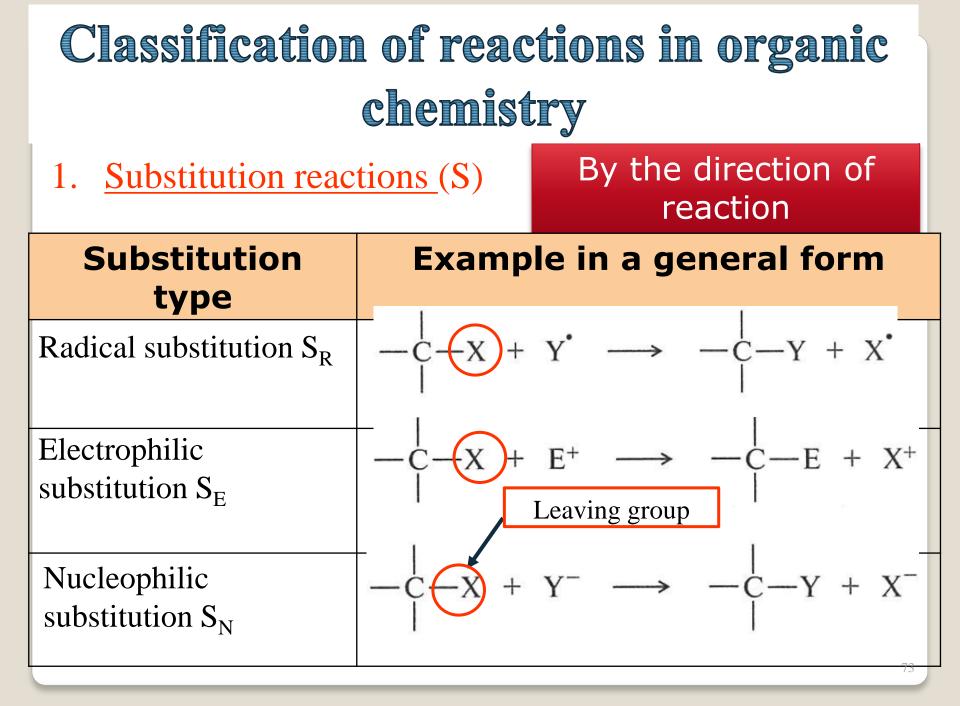
Reagent	Definition	Examples
Electrophile E+, E	A particle that forms a new covalent bond due to the partner's electronic pair.	H ⁺ , Br ⁺ , R ₃ C ⁺ , SO ₃ , AlCl ₃
<mark>Nucleophile</mark> Nu, Nu⁻	Particles forming a new covalent bond with a partner carrying a partial or full positive charge, providing their electron pair.	H ⁻ , Cl ⁻ , OH ⁻ , RO ⁻ NH ₃ , H ₂ O, CH ₂ =CH ₂ (alkenes), C ₆ H ₆ (arenes)

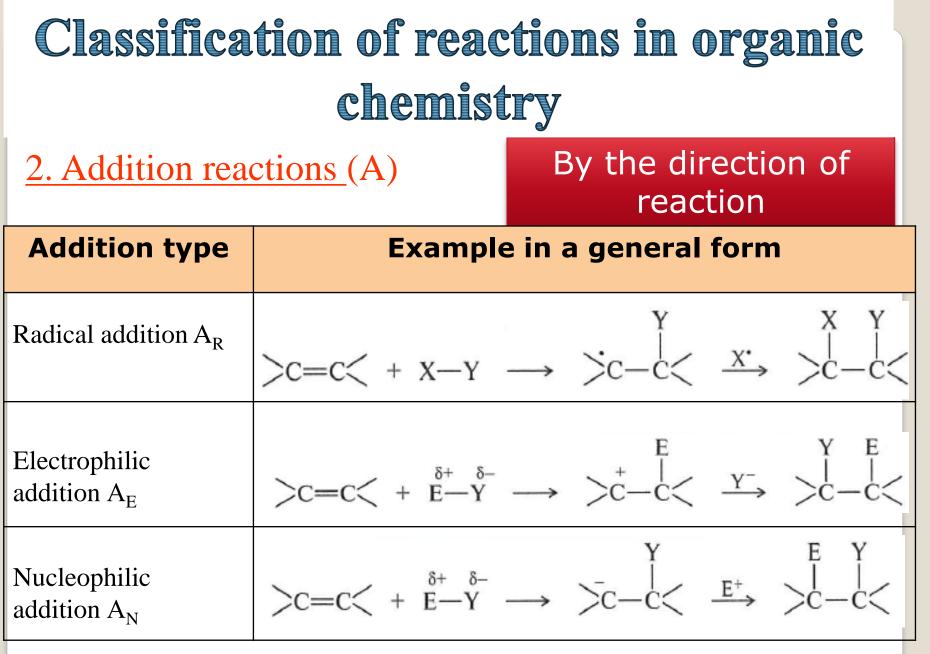


Reagent	Definition	Examples
Acid HA (BH ⁺)	Neutral molecules or ions capable of donating a hydrogen proton H ⁺ .	HC1, HC≡CH, CH ₃ COOH, NH ₄ ⁺ , H ₃ O ⁺
Base B, B⁻	Neutral molecules or "-" charged particles capable of tearing a proton away from an acid site.	OH^- , RO^- NH_3 , H_2O , $R-OH$, $R-NH_2$, $CH_2=CH_2$ (alkenes)



Reagent	Definition	Examples
Radical ·R	Free atom or particle with unpaired ē	·Cl, ·Br, ·OH, ·CH ₃
Oxidizer [O]	Neutral molecule or ion that accepts ē	O ₂ Fe ³⁺
Reducing agent [H]	Neutral molecule or ion that gives off ē	H ₂ , Fe ²⁺



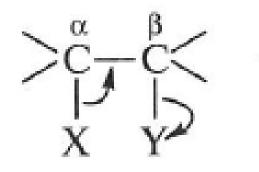


Classification of reactions in organic chemistry

3. Elimination reactions (E)

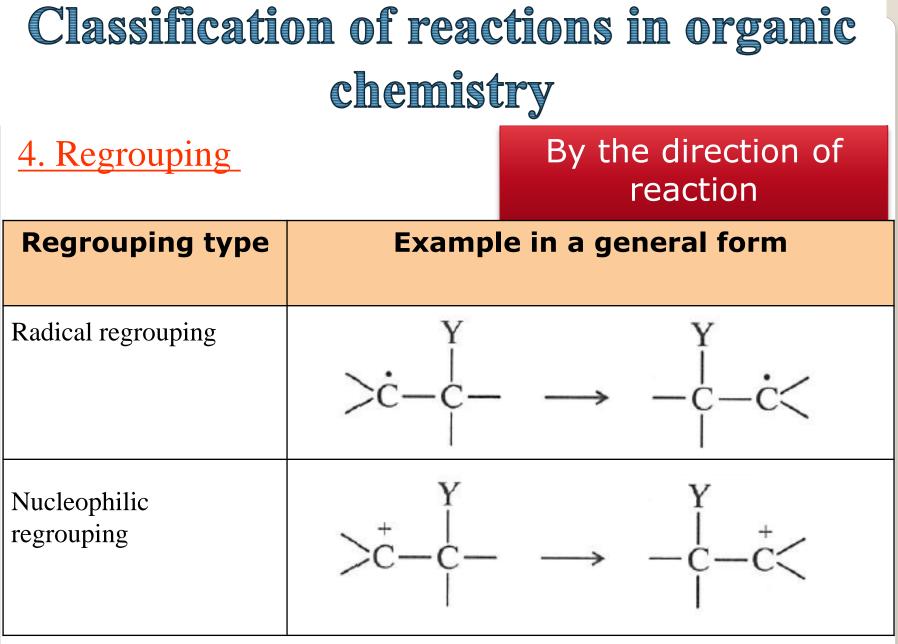
By the direction of reaction

Example in a general form



 $X + X^{+} + Y^{-}$

• Groups X and Y can leave sequentially or simultaneously, unite or not unite



Classification of reactions in organic chemistry

5. Redox reactions

By the direction of reaction

In the course of these reactions, the oxidation state of the carbon atom, which acts as a reaction center, changes.

Oxidation of organic compounds is the process of removing hydrogen to form a multiple bond or a new bond between a carbon atom and a heteroatom. Reduction is the reverse process of oxidation.

Redox series

