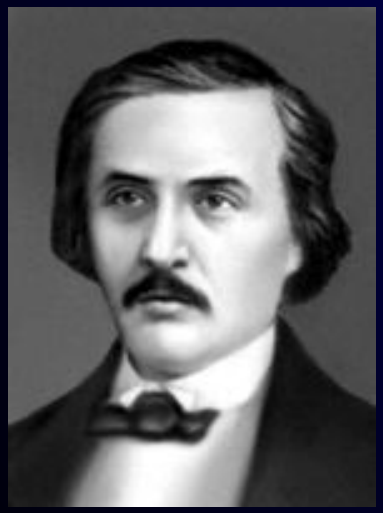
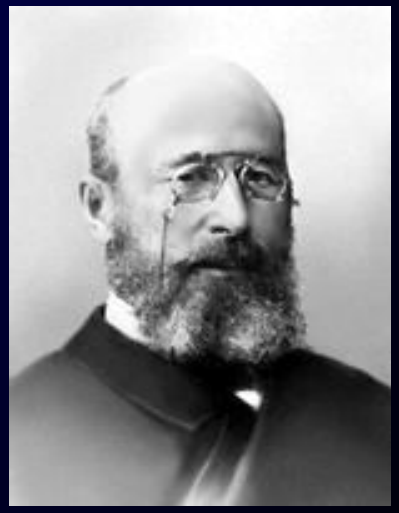
Lecture 1

Introduction in bioorganic chemistry. Isomerism and structure of organic compounds.

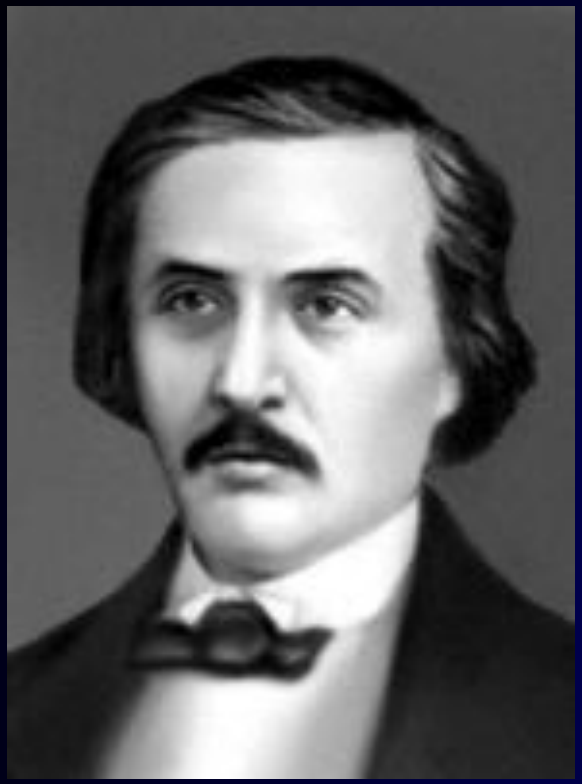




Organic chemistry — *chemistry of carbon containing compounds*

Elements **H**, **O**, **N**, **S**, P – organigenic elements

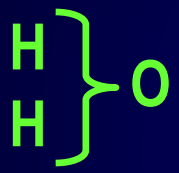
Bioorganic chemistry— *scientific discipline that combines organic chemistry and biochemistry*. **In most cases bioorganic chemistry deals with the** study of biological processes using chemical methods. (Wiki)



Charles Frédéric Gerhardt (21 August 1816 – 19 August 1856). French chemist, known for his work on reforming the notation for chemical formulas

In1853 C. Gerhardt elaborated «theory of the types» and use it for classification of organic compounds. According to Gerhardt theory, more complicated organic compound may be prepared on the basis of following “basic” types of the compounds

Hydrogen type

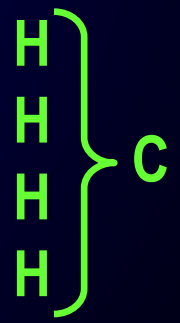


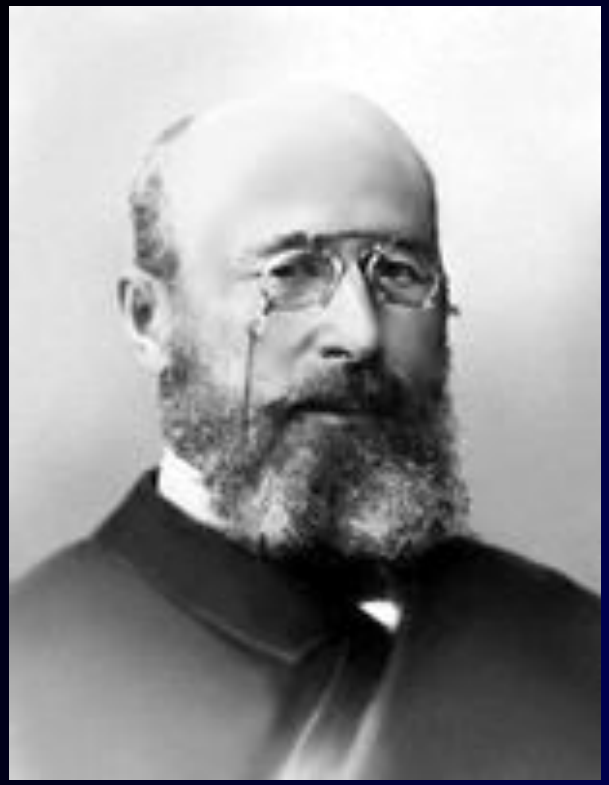
Water type

chlorine hydride type

Ammonia type

From **1857** on the proposal of **August Kekulé** hydrocarbons belong to the methane type





Alexander Mikhaylovich Butlerov (September 15, 1828 – August 17, 1886) - a Russian chemist, one of the creators of the theory of chemical structure

Basic statements of structure theory of organic compounds(1861)

1) In organic molecules atoms connected to each other according to their valences;

2) In organic molecules atoms bonded to each other in appointed order, what caused the chemical structure of molecule;

3) Chemical properties of organic molecules caused not only by quantity and nature of atoms, but on chemical structure of molecule.

Basic statements of structure theory of organic compounds(1861)

4) In organic molecules exists mutual effects between as bonded, so non-bonded atoms;

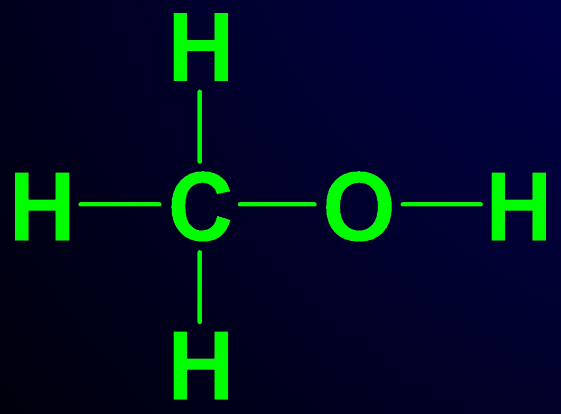
5) Chemical structure of organic compounds may be defined by its chemical transformations and chemical properties may be predicted from the structure.

Basic statements of structure theory of organic compounds(1861)

Structural formula – representation of bonds order in molecules

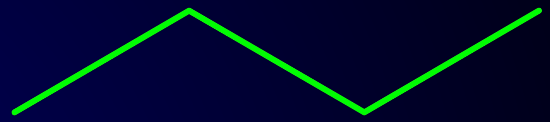
Empirical formula– CH_4O or CH_3OH

Structural formula



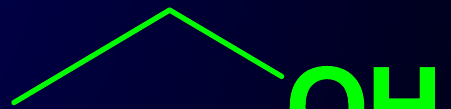
Structural formulas

$H_3C-CH_2-CH_2-CH_3$



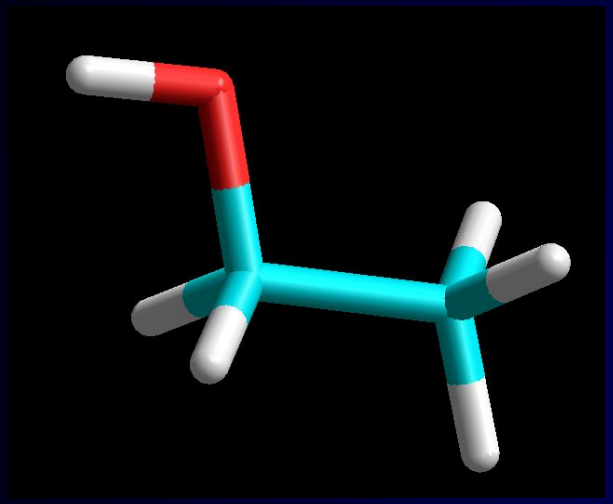
n-butane

H_3C-CH_2-OH

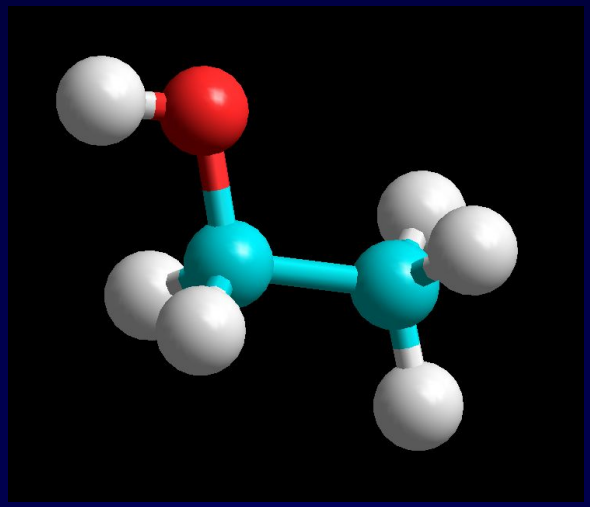


ethanol

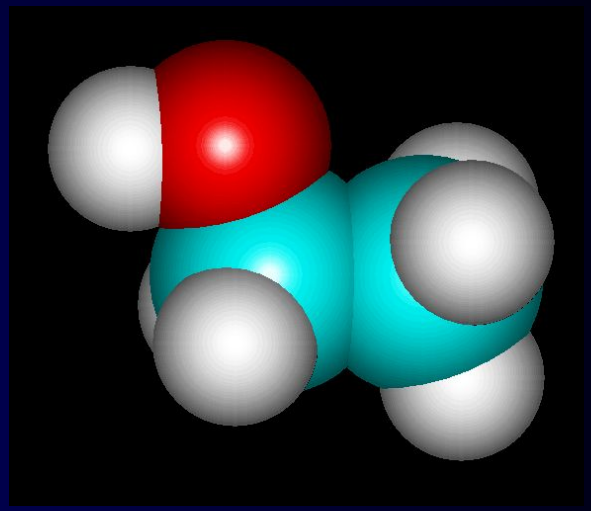
3D-models of organic compounds



Sticks

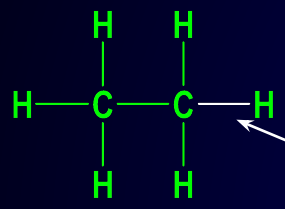


Ball & Stick



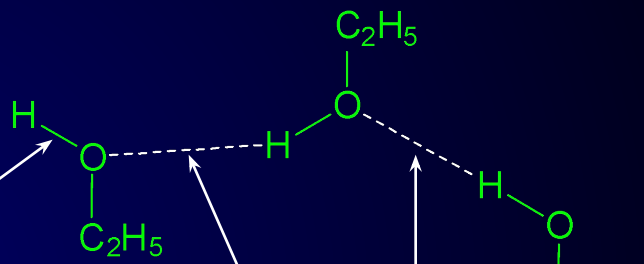
spherical

Bond types



Ethane

covalent bond



Ethanole

hydrogen bond

Ionic bond

sodium acetyl((4-aminophenyl)sulfonyl)amide

Covalent bond in organic molecules:

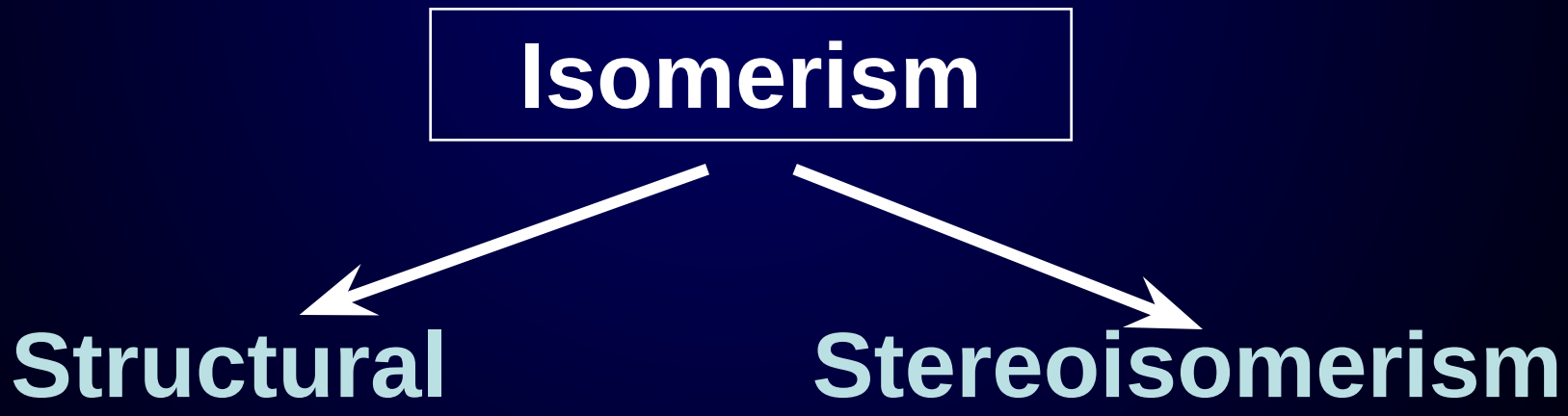
- Polar
- Non-polar
- Single (σ-bond)
- Double or triple (σ-bond and π-bond)

Hydrogen bond in organic molecules:

- Intermolecular
- Intermolecular

Chemical properties of organic molecules caused not only by quantity and nature of atoms, but on chemical structure of molecule.

Isomerism – phenomenon of existence of individual chemical compounds with the same qualitative and quantitative composition, but different structure and properties.



Structural isomerism caused by difference order and bonding type of atoms

- **Chain isomerism**
- **Position isomerism**
- **Functional group isomerism**
- **Tautomerism (dynamic isomerism)**

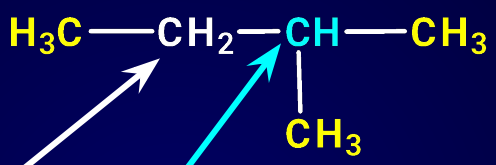
Изомерия цепи

n-Pentane

primary atoms

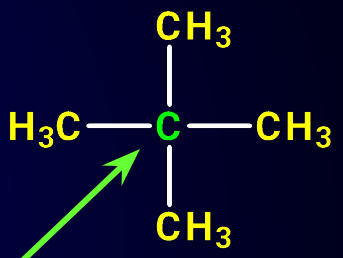
secondary atoms

iso-Pentane

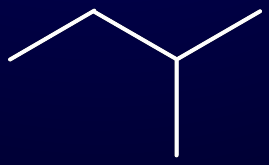


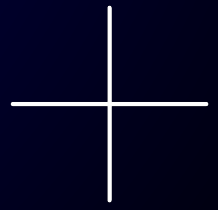
tertiary atoms

neo-Pentane



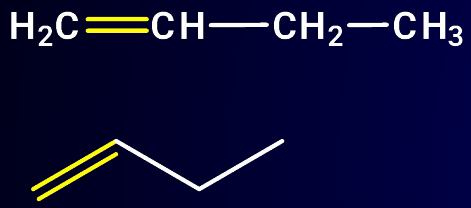
Quatemary atoms



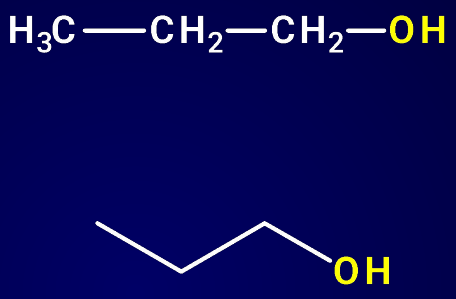


Positional isomerism

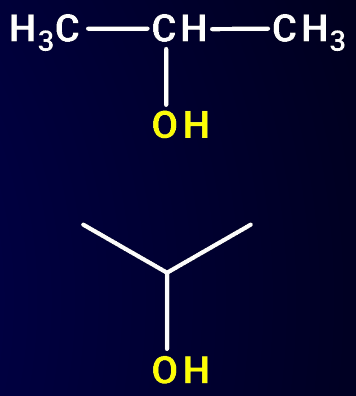
Butene-1



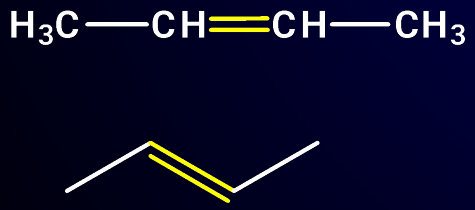
Propanol-1



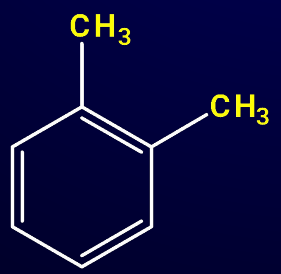
Propanol-2



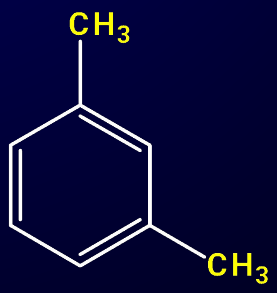
Butene-2



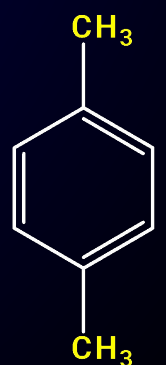
1,2-dimethylbenzene (o-xylene)



1,3-dimethylbenzene (u-xylene)



1,4-dimethylbenzene (p-xylene)



Functional group

- atom or group of atom which contain elements differ from carbon and hydrogen and reveals the same properties independent on location in molecule

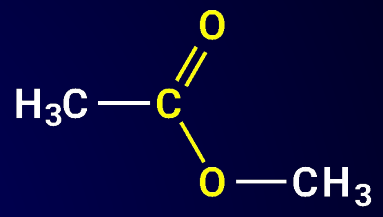
Functional group isomerism

C_2H_6O

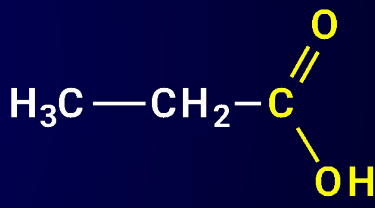
$H_3C—O—CH_3$ ether

$H_3C—CH_2—OH$ alcohol

$C_3H_6O_2$

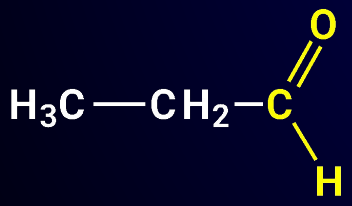


ester



carboxylic acid

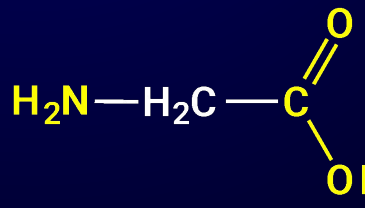
C_3H_6O



aldehyde

$H_3C—C(=O)—CH_3$ ketone

$C_2H_5NO_2$

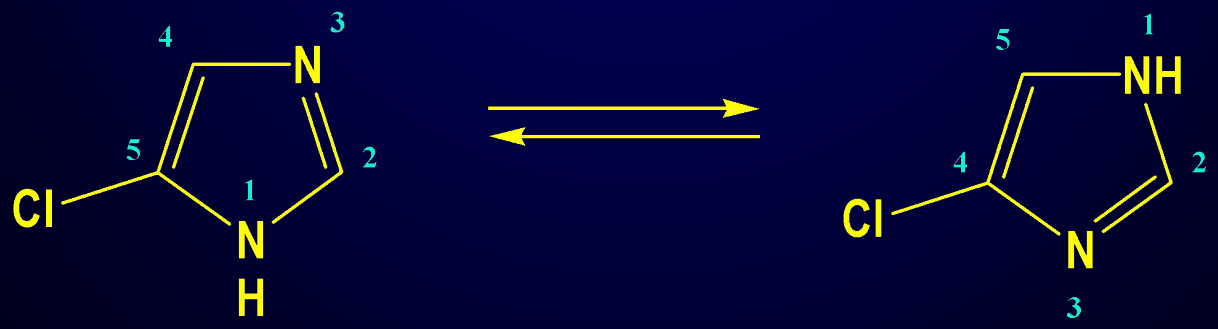


aminoacid

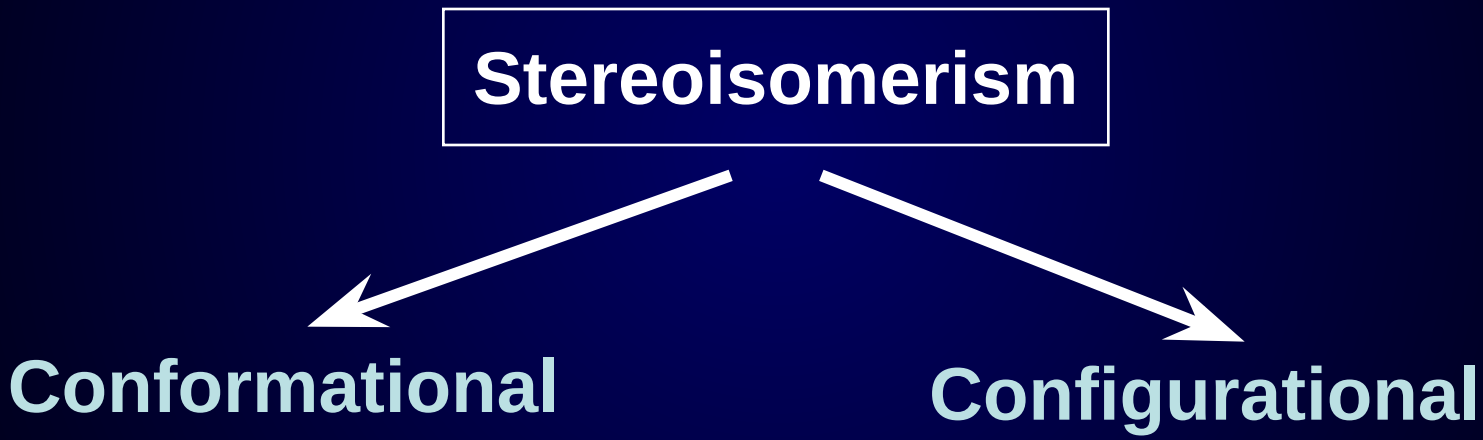
$H_3C—CH_2—NO_2$ nitroalkan

Tautomerism (dynamic isomerism)

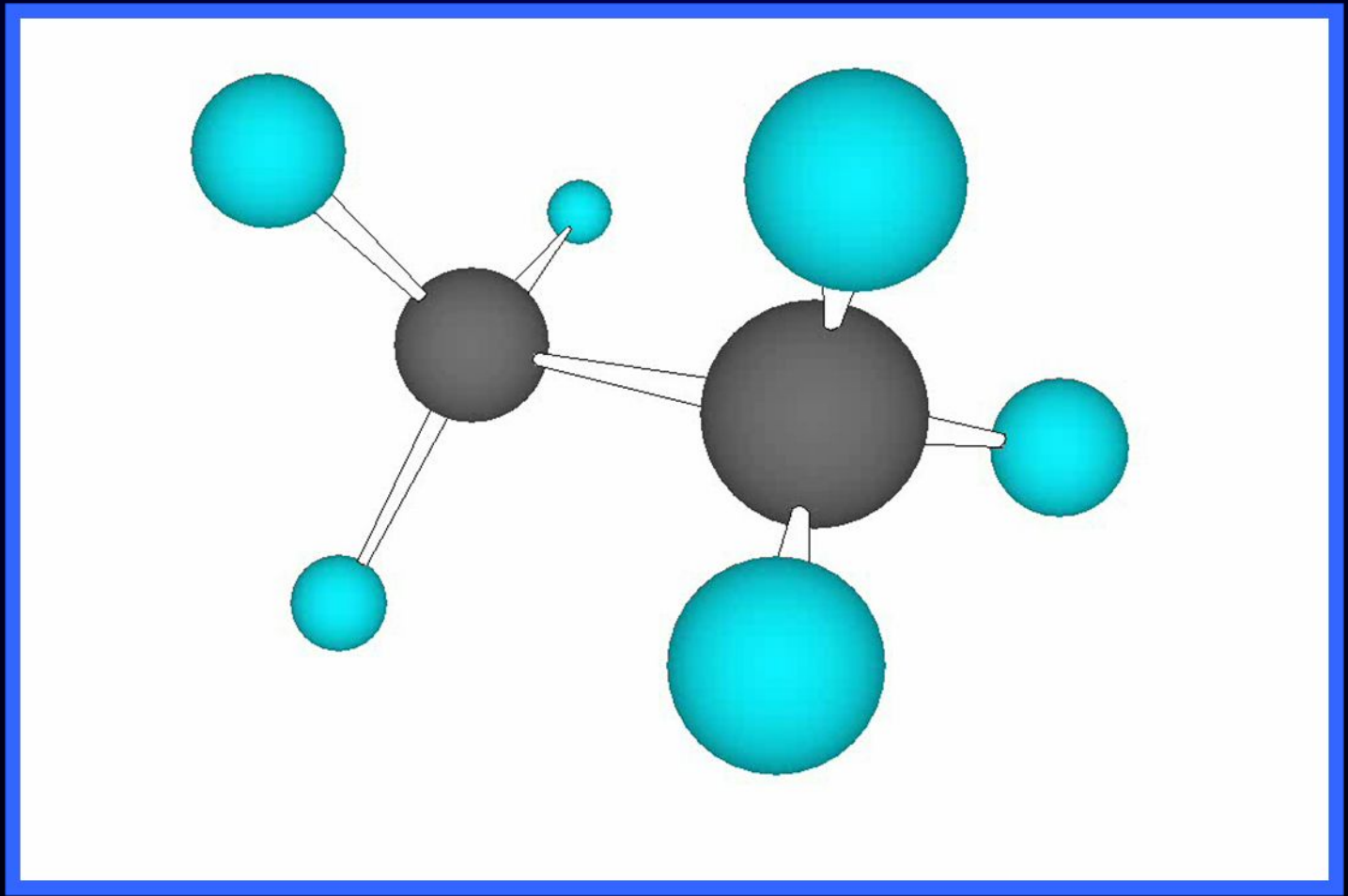
- Keto-enol
- Lactim-lactam
- Thion-thiol
- Ring-chain
- azole



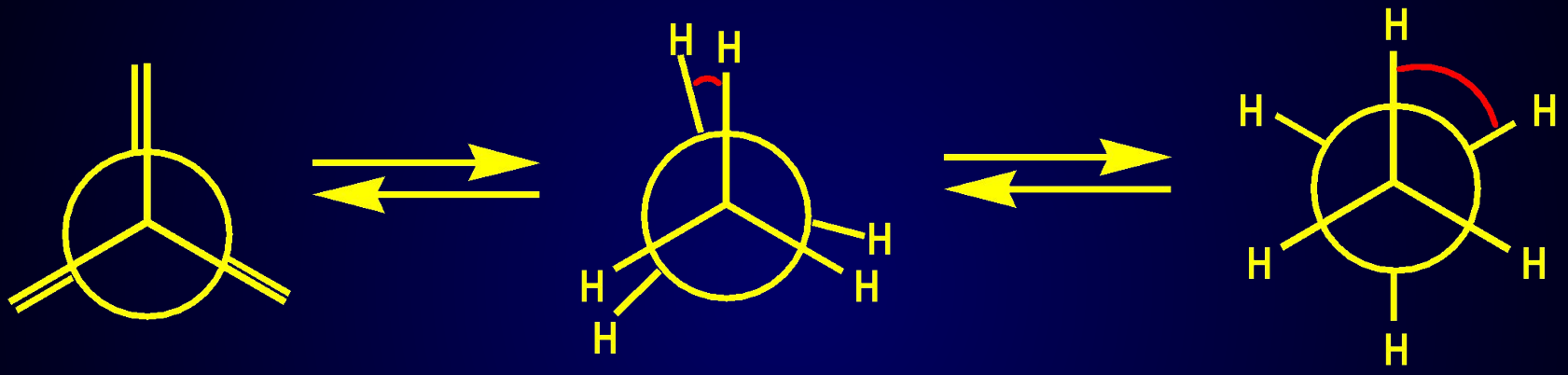
Stereoisomers are isomeric molecules that have the same molecular formula and sequence of bonded atoms (constitution), but that differ only in the three-dimensional orientations of their atoms in space



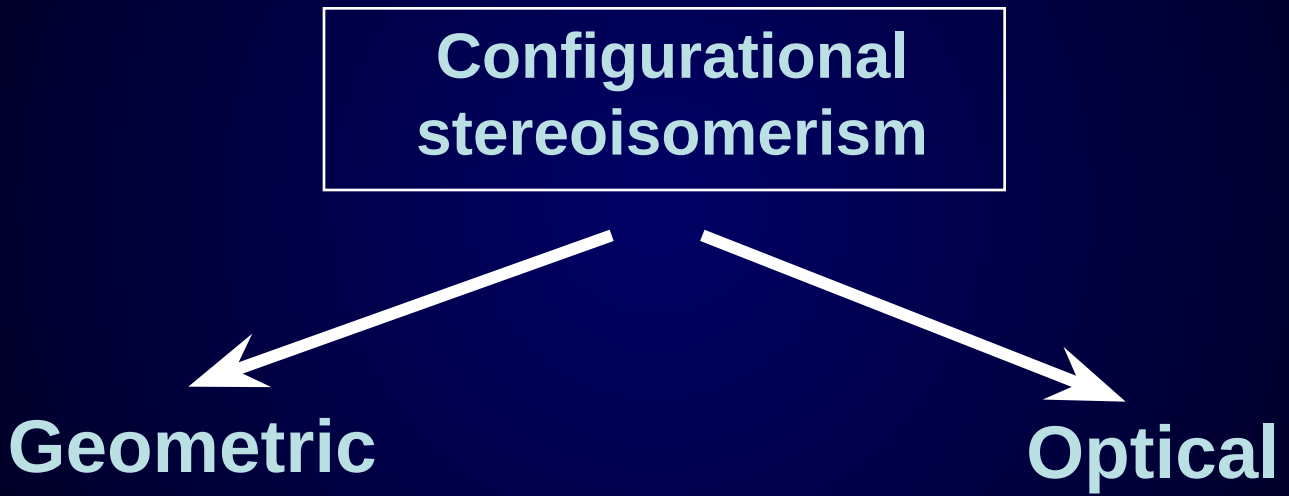
Conformational stereoisomerism caused by difference location of molecular fragments caused by the rotation about single bond



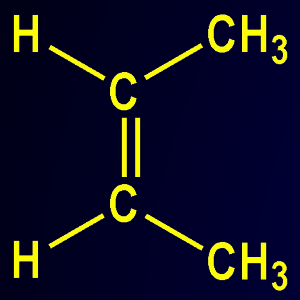
Conformations types



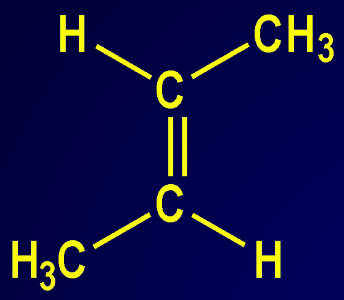
Configurational stereoisomerism caused by different location of atoms or group of atoms relative to “steric center” of molecule (asymmetrical carbon, double bond, cyclic system)



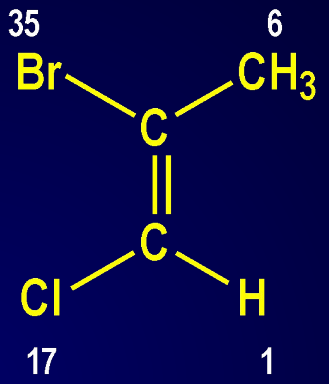
Geometric isomerism (cis-trans, E-Z-isomerism)
Caused by difference location of atoms and groups of atoms relative to plane of double bond or cycle.



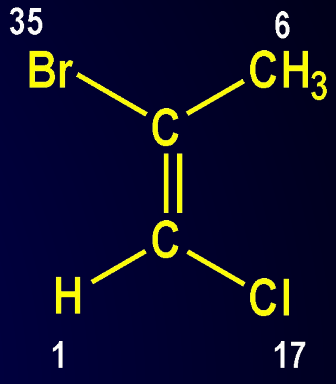
cis-buten-2



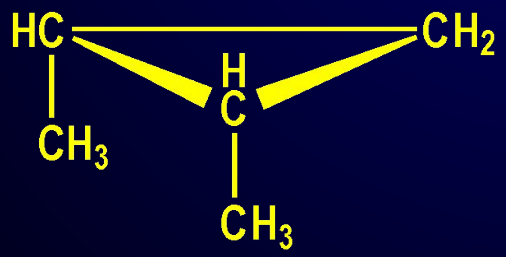
trans-buten-2



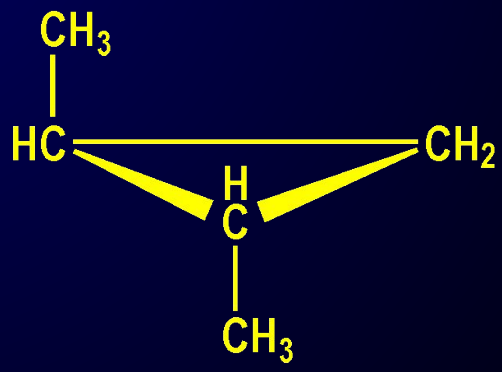
Z-isomer



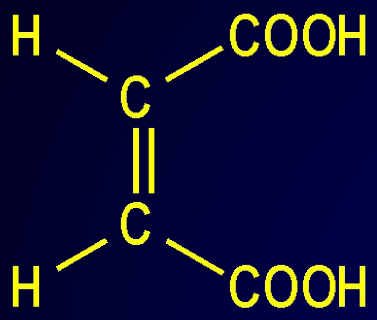
E-isomer



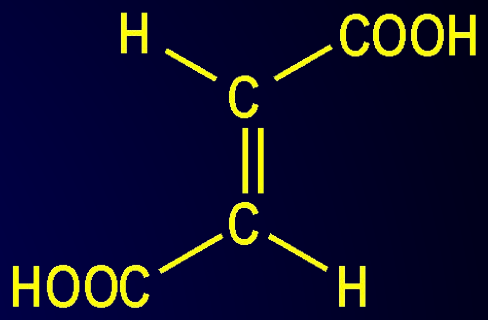
cis-1,2-dimethylcyclopropane



trans-1,2-dimethylcyclopropane

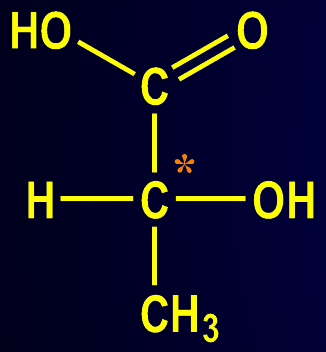


cis-butendioic acid,
maleic acid
Toxic compound



trans-*butendioic acid,*
maleic acid
Nontoxic compound

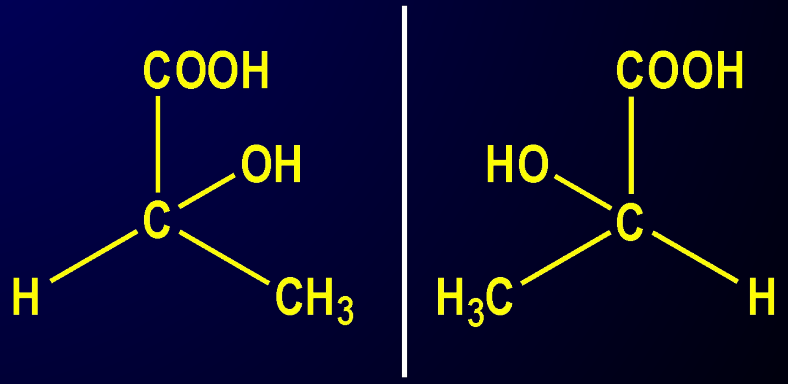
Optical isomerism caused by the presence in organic molecule carbon atom with four different substituent.



lactic acid

Chiral molecule may exists two enantiomers (mirror images)

Optically active compounds, such as slactic acid causes rotation of the polarization of plane polarized light as it passes through the sample.

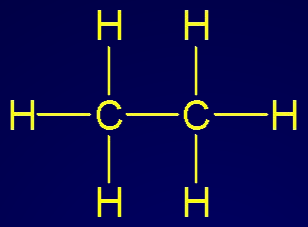


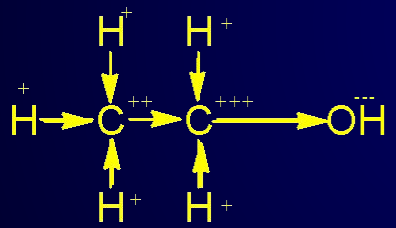
mirror plane

Thalidomide tragedy

Electronic effects in organic molecules

Inductive effect - transmission of charge through a chain of atoms in organic molecule. Mentioned transmission occurs on σ-bonds. Inductive effects are dumping.





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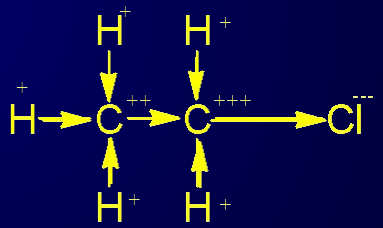

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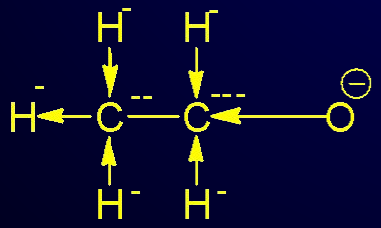

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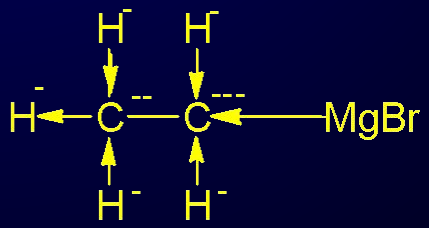

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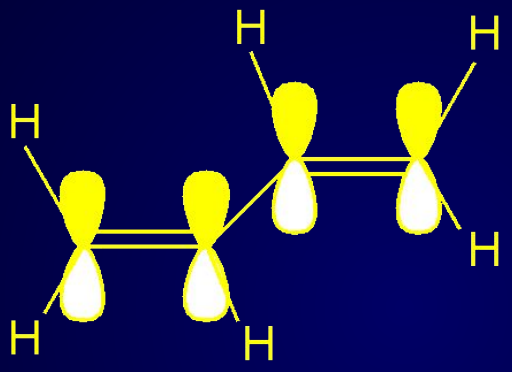
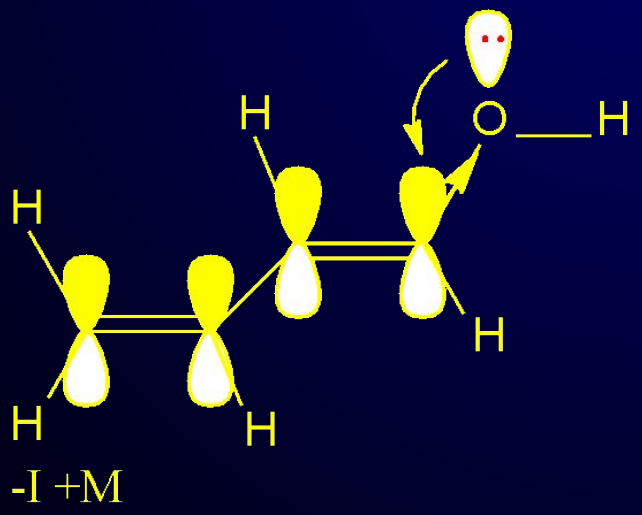
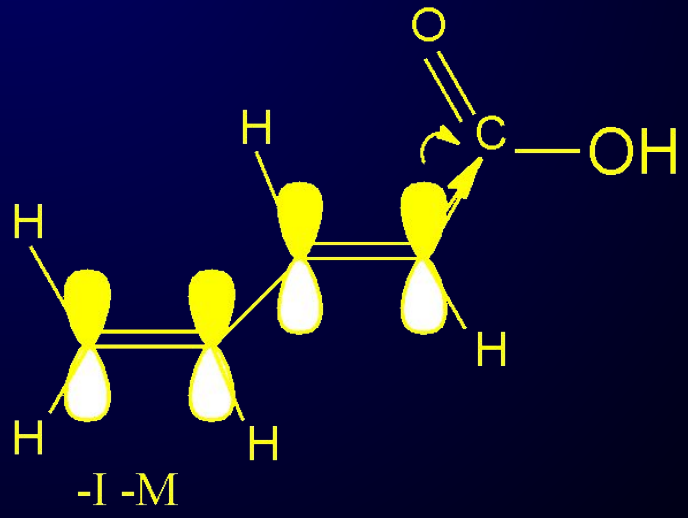
Electronic effects in organic molecules

Mesomeric effect - transmission of charge through a conjugated system in organic molecule. Mentioned transmission occurs on Mesomeric effects are not dumping.







Thank You for kind attention!