# Organic Chemistry Concepts LOKT.09.051

### Organic molecules 2

### **Topics**

- classes of compounds
  - functional groups
  - rules of naminmg

### Bond length (pm) and energy (kJ/mol)

Bond	Length	Energy	Bonde	Length	Energy
Н-Н	74	436	H-C	109	413
C-C	154	348	H-N	101	391
N-N	145	170	Н-О	96	366
O-O	148	145	H-F	92	568
F-F	142	158	H-Cl	127	432
Cl-C	1 199	243	H-Br	141	366
Br-B	r 228	193	H-I	161	298
I-I	267	151			

### Electronegativity scale

H						
2.1						
Li	Be	В	C	N	O	F
1.0	1.5	2.0	2.5	3.0	3.5	4.0
Na	Mg	Al	Si	P	S	Cl
0.9	1.2	1.5	1.8	2.1	2.5	3.0
0.9 K	1.2 Ca	1.5	1.8	2.1	2.5	3.0 Br

Proposed by L. Pauling

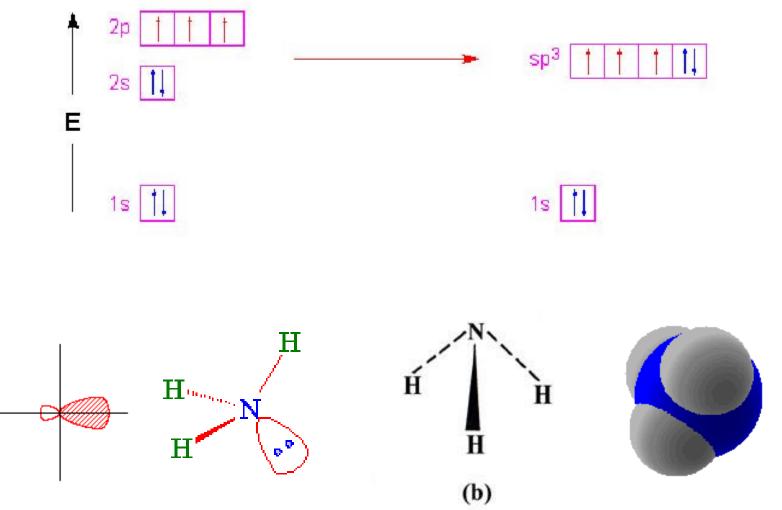
### Bond angles

• H-O-H 104°

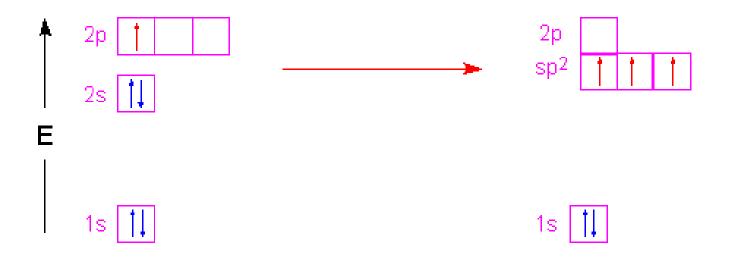
• C-O-H 107-109°

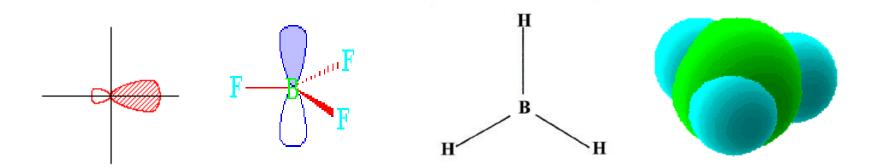
• C-O-C 111º

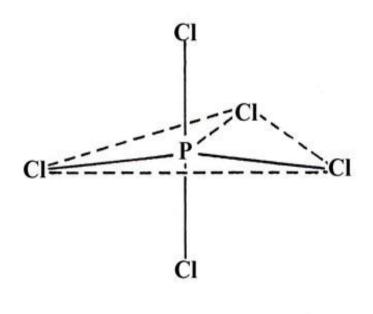
### Electron configuration of nitrogen atom



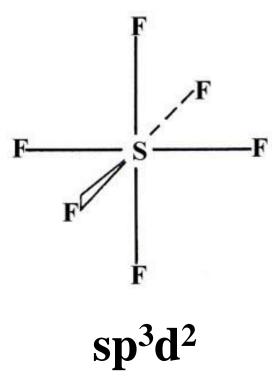
### Electron configuration of boron atom











Geometry	Hybrid orbitals	Hybrid name
LINEAR	2	s <b>p</b>
PLANAR	3	$sp^2$
TETRAHEDRAL	4	sp <sup>3</sup>
BIPYRAMIDAL	5	$sp^3d$
OCTAHEDRAL	6	$sp^3d^2$

## Drawing and naming of organic molecules

 Organic molecules have backbone formed by chain of carbon atoms and drawing and naming are based on this fact

- Nomenclature enables translation of name into structure and naming a molecule from its structure
- This is coding and decoding problem

### **Functional group coding**

Functional group	code
Halide	halogeno-
Amine	Amino-
Alcohol	-ol
Aldehyde	-al
Ketone	-one
Carboxylic acids	-oic acid
Carboxylic acids, esters and salts	-oate
Amide	-amide

### Drawing organic molecules

- Molecular formulae ( C<sub>2</sub>H<sub>6</sub>O)
- Structural formulae (2D)
  - Extended
  - Condensed
  - Bond-line structure (skeletal structure)
- 3D presentation

### Modeling organic molecules

- Stick model, showing bond direction
- Ball and stick model showing atoms
- Space-filling model showing bulk molecules

http://orgaanilinekeemia.ee/molekulide-andmebaas/

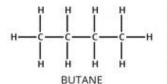
### • TYPES OF ISOMERISM IN ORGANIC CHEMISTRY •

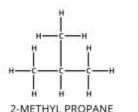
A GUIDE TO THE FIVE MAIN TYPES OF ISOMERISM THAT CAN BE EXHIBITED BY ORGANIC COMPOUNDS

AN ISOMER OF A MOLECULE IS A MOLECULE WITH THE SAME MOLECULAR FORMULA BUT A DIFFERENT STRUCTURAL OR SPATIAL ARRANGEMENT OF ATOMS. THIS VARIATION CAN LEAD TO A DIFFERENCE IN PHYSICAL OR CHEMICAL PROPERTIES.

#### STRUCTURAL ISOMERISM

#### CHAIN

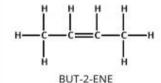


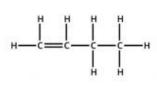


#### DIFFERENT ARRANGEMENT OF A MOLECULE'S CARBON SKELETON

The positions of the carbon atoms in the molecule can be rearranged to give 'branched' carbon chains coming off the main chain. The name of the molecule changes to reflect this, but the molecular formula is still the same.

#### POSITION



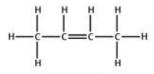


### THE DIFFERING POSITION OF THE SAME FUNCTIONAL GROUP IN THE MOLECULE

BUT-1-ENE

The molecular formula remains the same; the type of functional group also remains the same, but its position in the molecule changes. The name of the molecule changes to reflect the new position of the functional group.

#### FUNCTIONAL



BUT-2-ENE



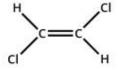
CYCLOBUTANE

#### DIFFERING POSITIONS OF ATOMS GIVE A DIFFERENT FUNCTIONAL GROUP

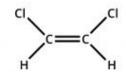
Also referred to as functional group isomerism, these isomers have the same molecular formula but the atoms are rearranged to give a different functional group. The name of the molecule changes to reflect the new functional group.

#### STEREOISOMERISM

#### GEOMETRIC



(E)-1,2-DICHLOROETHENE E = opposite side

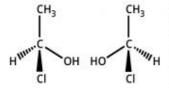


(Z)-1,2-DICHLOROETHENE Z = same side

#### DIFFERENT SUBSTITUENTS AROUND A BOND WITH RESTRICTED ROTATION

Commonly exhibited by alkenes, the presence of two different substituents on both carbon atoms at either end of the double bond can give rise to two different, nonsuperimposable isomers due to the restricted rotation of the bond.

#### **OPTICAL**



L: (S)-1-CHLOROETHANOL R: (R)-1-CHLOROETHANOL



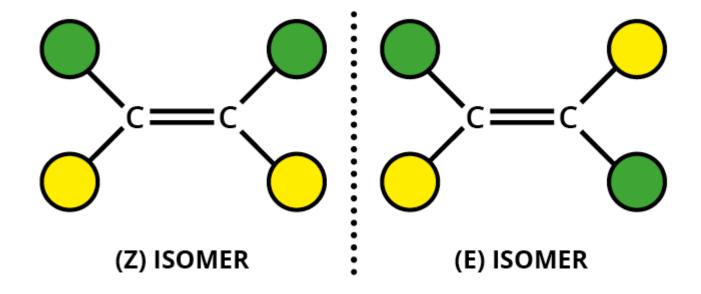


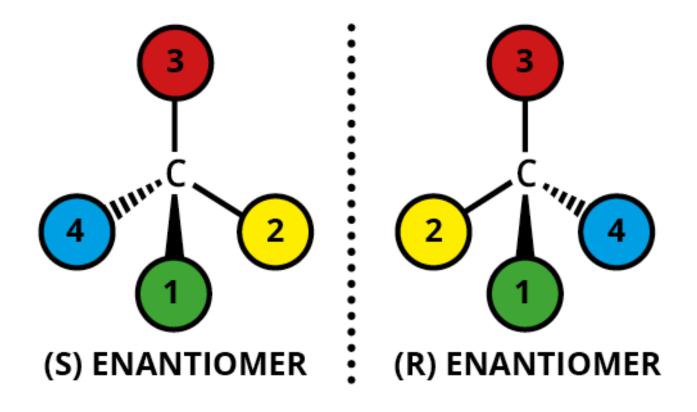
#### NON-SUPERIMPOSABLE MIRROR IMAGES OF THE SAME MOLECULE

Optical isomers differ by the placement of different substituents, around one or more atoms in a molecule. Different arrangements of these substituents can be impossible to superimpose - these are optical isomers.









### **HOMEWORK**

### **CHAPTERS 2 AND 3**

ROOS, G, ROOS, C, ORGANIC CHEMISTRY CONCEPTS, ACADEMIC PRESS 2015,