



PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	Name
QO321	Organic Chemistry I

Vector
OF:S-5 T:004 P:000 L:000 O:000 D:000 HS:004 SL:004 C:004 AV:N EX:S FM:75%

Pre requirement
QG101 QG102/ QG108

Summary
Introduction to the discipline: some historical aspects and structural theory. Electronic Structure and Chemical Bonding. Organic Structures. Organic Reactions. Alkanes. Reactions of alkanes. Stereochemistry. Alkyl halides and organometallic. Structure and physical properties of alkyl halides. Uses of halogenated hydrocarbons, nomenclature and structure of organometallic substances, physical properties and preparation of organometallic, organometallic reactions. Nucleophilic substitution and eliminations. Alcohols and ethers. Alkenes. Alkynes and nitriles.

Program
<ol style="list-style-type: none">1. Introduction to the discipline: Organic chemistry as science, some historical aspects and structural theory.2. Electronic Structure and Chemical Bonding:<ol style="list-style-type: none">a) Structural theory of organic chemistry;b) Chemical bonds, octet rule;c) Lewis structures, formal charge;d) Resonance structures;e) Atomic orbitals and molecular orbitals;f) Hybrid orbitals and their connections;g) Molecular geometry.3. Organic compounds<ol style="list-style-type: none">a) Functional groups;b) Chemical bonds: apolar and polar covalent bonds, electronegativities, dipoles;c) Intermolecular interactions.4. Introduction to organic reactions. Acidity and basicity<ol style="list-style-type: none">a) Examples of organic reactions, equilibrium.b) Acid-base reactions, Bronsted and Lewis acids and bases;c) The strength of acids and bases, K_a and pK_a;d) Acid-base equilibrium;e) Relationship between acidity-basicity and structure.

5. Alkanes

- a) n-Alkanes: nomenclature, physical properties;
- b) n-Alkanes: rotation barriers along the C-C bonds, conformations;
- c) Branched alkanes;
- d) Cycloalkanes: ring tension, torsional tension and steric tension, cycloalkane conformations;
- e) Heat of Formation and bond dissociation energy;
- f) Occurrence of alkanes;
- g) Reactions of alkanes: pyrolysis; radical halogenation, radical stability, combustion.

6. Stereochemistry

- a) Isomerism: constitutional isomers and stereoisomerism;
- b) Chirality, importance of chirality in biological systems;
- c) Enantiomers
- d) Nomenclature of enantiomers: the R and S system
- e) Properties of chiral molecules: optical activity, optical purity;
- f) Racemates;
- g) Substances containing more than one stereocenter: diastereoisomers;
- f) Fischer projections;
- g) Stereochemistry in cyclic systems;
- h) Prochiral faces: face Re and face Si;
- i) Chemical reactions and stereoisomerism.

7. Alkyl halides. Nucleophilic substitution and eliminations

- a) Structure and properties of alkyl halides;
- b) Use of halogenated hydrocarbons, dipoles, polarizability;
- c) The substitution reaction: nucleophiles, electrophiles, leaving group;
- d) SN2 reaction: mechanism, free energy diagram; transition state;
- e) The effect of the alkyl halide structure on the substitution process;
- f) The effect of the nucleophile structure on the substitution process; basicity and nucleophilicity;
- g) The effect of the solvent;
- h) The effect of the output group;
- i) SN1 reaction: mechanism; transition states and intermediates, free energy diagram;
- j) Stability of carbocations;
- k) Elimination reactions and temperature effect; competitive reactions;
- l) Substitution and elimination reactions in cyclic systems.

8. Alkenes and alkynes

- a) Electronic structure; nomenclature, stereoisomerism: E and Z system in alkenes; physical properties;
- b) Relative stability of alkenes: heat of hydrogenation
- c) Cycloalkenes, relative stability;
- d) Preparation of alkenes: elimination reactions E2 and E1, dehydrohalogenation, dehydration;
- e) Preparation of alkynes: dehalogenation of vicinal and geminal halides. Alkynes reactions. Acidity and use in carbon-carbon bond formation reactions;
- f) Reactions of alkenes and alkynes: addition of syn and anti hydrogens;
- g) Addition reactions: additions of alkyl halides, Markovnikov rule, addition stereochemistry; hydration, rearrangement of carbocations; addition of halogens, stereochemistry; regioselective reactions; formation of halohydrins;

h) Oxidation: dihydroxylation, oxidative cleavage, epoxidation; formation of cyclopropanes: carbenes.

9. Alcohols and Ethers

a) Structure, nomenclature and physical properties of alcohols and ethers. Industrial sources of most common alcohols;

b) Acidity of alcohols;

c) Preparation of alcohols: transformation of functional groups; formation of new carbon skeletons;

d) Reactions of alcohols: eliminations, substitutions, additions, oxidations;

e) Preparation of ethers;

f) reactions of ethers;

g) Cyclic ethers, epoxides.

Bibliography

1. Solomons, G.; Fryhle, C. "Organic Chemistry", 8th ed., 2004; John Wiley & Sons Inc.: NY;
2. Streitwieser, A.; Heathcock, C.H.; Kosower, E.M. "Introduction to Organic Chemistry", 4th ed., 1992; MacMillan Publis. Comp.: NY;
3. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P. "Organic Chemistry", 2004; Oxford Univ. Press: Oxford;

Carey, F. A. "Organic Chemistry", 5th ed., 2003; McGraw-Hill, Inc.: NY.

Evaluation criteria

For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures.

For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.