UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	**Name**
QO427	Organic Chemistry I

Vector
OF:S-2 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

Summary

Hybrid orbitals. Hydrocarbons. Petroleum. Benzene and derivatives. Organic halides. Alcohols. Ethers. Carboxylic acids and derivatives. Aldehydes and ketones. Amines. Heterocyclic compounds. Polymers. Notions of Stereochemistry.

Program

1. Introduction to the discipline: Organic chemistry as a science, some historical aspects and structural theory.

2. Electronic Structure and Chemical Bonding:

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;

f) Molecular geometry.

3. Organic compounds

a) Functional groups;

b) Chemical bonds: nonpolar and polar covalent bonds, electronegativities, dipoles; intermolecular interactions.

4. Introduction to organic reactions. Acidity and basicity

a) Examples of organic reactions, equilibria.

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 energy of bond dissociation;

f) Occurrence of alkanes;

g) Reactions of alkanes: pyrolysis; radical halogenation, radical stability, combustion.

h) Petroleum.

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:*Re* and *Si*faces;

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 groups;

d) S_N2 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 leaving group;

i) S_N1 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: system *E* and *Z* in alkenes; physical properties;

b) Relative stability of alkenes: hydrogenation heats

c) Cycloalkenes, relative stability;

d) Preparation of alkenes: elimination reactions E2 and E1, dehydroalogenation, dehydration;

e) Preparation of alkynes: dehalogenation of vicinal and geminal halides. Alkyne 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.

i) Polymers: main classes of polymers and polymerization reactions.

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) ethers reactions;

g) Cyclic ethers, epoxides.

10. Aldehydes and ketones.

a) Structure and Properties.

b) Occurrence and use.

c) Description of the carbonyl group by valence theory and molecular orbitals theory.

d) General methods of preparation of aldehydes and ketones.

e) Addition of oxygen and nitrogen nucleotides to aldehydes and ketones: formation of hydrates, ketals and hemiketals, imines, enamines and related compounds.

f) Addition of carbon nucleophiles: hydrocyanic acid, organometallic reagents (Grignard reaction), phosphorus ylides (Wittig reaction) and phosphonates.

g) The influence of substituents on the reactivity of aldehydes and ketones.

h) Stereochemical aspects of the addition of nucleophiles to aldehydes and ketones.

i) Methods of aldehyde and ketone oxidation and reduction: Baeyer-Villiger oxidation, Cr (VI) oxidation, reduction by metal hydrides, catalytic hydrogenation, Clemmensen reaction, Wolff-Kischner reaction.

11. Carboxylic acids.

a) Structure and properties.

b) Occurrence and use.

c) Acidity.

d) Inductive and electronic effects on the acidity of carboxylic acids.

e) Formation of salts, soaps, detergents and surfactants.

f) Esterification reactions.

g) Formation of acyl halides, anhydrides, esters and amides.

h) Reduction of the carboxylic group.

12. Carboxylic acid derivatives: esters, amides, acyl halides, carboxylic acid anhydrides.

a) Structure and properties.

b) Occurrence and use.

c) Description by valence bond theory and molecular orbitals theory.

d) General mechanism of the addition of nucleophiles to carboxylic acids and derivatives.

e) The hydrolysis reaction.

g) Possible reactions of interconversion of derivatives.

h) The acidity of alpha hydrogen in carboxylic acids and derivatives.

i) Enolate formation, alkylation reaction and aldol reaction.

j) The addition of organometallic to carboxylic acids and derivatives.

13. Benzene and derivatives.

a) Historical aspects.

b) Structure, nomenclature and properties.

c) The resonance energy.

d) Description by valence bond theory and molecular orbitals theory.

e) The Hückel rule.

f) Reactions in the side chains of aromatic compounds: S_N2, S_N1, hydrogenolysis, oxidation.

g) Birch reduction.

14. Electrophilic aromatic substitution reactions

a) Halogenation, nitration, sulfonation, alkylation and Friedel-Crafts acylation reactions. b) Orientation effects in S_EAR.

c) Effects of multiple substituents.

15. Amines

a) Structure and properties.

b) Sources and use.

c) Basicity and formation of salts.

d) Formation of imines and enamines.

e) Methods of preparation: alkylation, reduction of nitro compounds, nitriles, azides, imines and oximes.

f) Reductive amination.

g) The Hofmann and Curtius rearrangements.

h) Formation of diazonium salts.

16. Heterocyclic compounds: examples, properties and syntheses.

Bibliography

F. A. Bettelheim, W. H. Brown, J. March, "Introduction to General, Organic & Biochemistry", Harcourt College Publishers, 6th ed., 2001, Philadelphia.
R.C. Atkins and F.A. Carey, "Organic Chemistry - A Brief Course", 1990, McGraw-Hill Public. Co.
L. C. de A. Barbosa "Introdução à Química Orgânica", Ed. UFV., Pearson Prentice Hall, 2004.
J. McMurry, "Organic Chemistry", Thomson Learning Ltda., 6a. Ed., 2005.
Bruice, P. Y., "Organic Chemistry", Pearson Prentice Hall, S. Paulo, 4a. Ed., 2006.
T. W. G. Solomons, Química Orgânica, Livros Técnicos e Científicos Editora S.A., 1983.
Other authors: Morrison & Boyd; C. Heathcook e N. Allinger, among others.

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.