UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	**Name**
QO323	Organic Chemistry I (Chemical Engineering)

Vector
OF:S-1 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/QG107

Summary

Hydrid Orbitals. Hydrocarbons. Petrol. Benzene and derivatives. Organic halides. Alcohols. Ethers. Carboxylic acids and derivatives. Aldeydes and ketones. Amines. Heterocyclic compounds. Polymers. Basic principles of stereochemistry.

Program

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

2. Eletronic structure and chemical bond:
a) Organic chemistry structural theory;
b) Chemical bonds, octet rule;
c) Lewis structures, formal charge;
d) Resonance structures;
e) Atomic and molecular orbitals;
f) Hydrid orbitals and their bonds;
g) Molecular geometry.

3. Organic compounds
a) Functional groups;
b) Chemical bonds: non polar and polar covalent bonds, electronegativity and dipoles;
c) Intermolecular interactions.

4. Introduction to the organic reactions. Acidity and Basicity.
a) Examples of organic reactions, chemical equilibra.
b) Acid-base reactions, Brønsted acids and bases;
c) Acids and bases strenghts, K_a and pK_a;
d) Acid-base equilibrium;
e) Acidity-basicity and structure relationship.

5. Alkanes
a) n-Alkanes: nomenclature, physical properties;
b) n-Alkanes: rotation barriers along C-C bonds, conformations;
c) Branched alkanes;
d) Cycloalkanes: ring tension, sterical and torsional tensions, cycloalkanes conformations;
e) Formation heats and bond dissociation energies;
f) Alkanes occurrence;
g) Alkane reactions: pyrolisis; radical halogenation, radical stability, combustion.
h) Petrol.

6. Stereochemistry

a) Isomerism: constitutional isomers and stereoisomerism;
b) Chirality, importance in biological system;
c) Enantiomers
d) Enantiomers nomenclature: R and S system
e) Properties of chiral molecules: Optical activity and purity;
f) Race mates;
g) Substances containing more than one stereocenter: diastereoisomers;
f) Fisher projections;
g) Stereochemistry in cyclic systems;
h) Pro-chiral faces: *Re* and *Si* faces;
i) Chemical reactions and stereoisomerism.

7. Alkylhalides. Nucleophilic substitutions and eliminations
a) Structure and property of alkylhalides;
b) Use of halogenated hydrocarbons, dipoles, polarizability;
c) Displacing reaction: nucleophiles, electrophiles, leaving groups;
d) S_N2 reaction: mechanism, free energy diagram; transition state;
e) The effect of alkylhalide structure in the displacing process;
f) The effect of the nucleophile structure in the displacing process; basicity and nucleophilicity;
g) Solvent effects;
h) Leaving group effects;
i) S_N1 reaction: mechanism; transition state and intermediates, free energy diagram;
j) Carbocations stability;
k) Elimination reactions and temperature effect; competitive reactions;
l) Substitution and Elimination in cyclic systems.

8. Alkenes e alkynes
a) Electronic structure; nomenclature, stereoisomeria: *E* and *Z* system in alkenes; physical properties;
b) Relative stability of alkenes: hydrogenation heats
c) Cycloalkenes, relative stability;
d) Preparaction of alkenes: E2 and E1 elimination reactions, dehydrohalogenation, dehydration;
e) Preparation of alkynes: dehydrohalogenation of vicinal and geminal halides. Alkyne reactions. Acidity and use in reactions of Carbon-Carbon bond formation;
f) Alkenes and alkynes reactions: *syn* and *anti* hydrogen additions;
g) Addition reactions: alkylhalides addition, Markovnikov rule, addition stereochemistry; hydration, carbocations rearrangements; halogens addition, stereochemistry; régio selective reactions; halohydrins formation;
h) Oxidations: di-hydroxylation, oxidative cleavage, epoxidation; cyclopropanes formation: carbenes.
i) Polymers: main classes of polymers and polymerization reactions.

9. Alcohols and Ethers
a) Structure, nomenclature and physical properties of alcohols and ethers. Most common industrial sources;
b) Alcohols acidity;
c) Preparation of alcohols: functional group transformations; formation of new carbon skeletons;
d) Alcohol reactions: eliminations, substitutions, additions, oxidations;
e) Ethers preparation;
f) Reactions of ethers;
g) Cyclic ethers and epoxides.

10. Aldehydes and Ketones.
a) Structure and Properties.
b) Occurrence and use.
c) Description of the carbonyl group by using the Valence and Molecular Orbital theories.
d) General methods for the preparation of aldehydes and ketones.
e) Additions of oxygen and nitrogen nucleophiles to aldehydes and ketones: hydrate formation, ketals and hemiketals, imines, enamines and related compounds.
f) Addition of carbono nucleophiles: hydrocyanic acid, organometallic reagents (Grignard

reactions), Phosphorylides (Wittig reaction) and phosphonates.
g) The influence of substituents on the reactivity of aldehydes and ketones.
h) Stereochemical aspects in the addition of nucleophiles to aldehydes and ketones.
i) Reduction and oxidation methods of aldehydes and ketones: Baeyer-Villiger oxidation, oxidation with Cr(VI) reagents, metal hydrides reduction, 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 carboxylic acid acidity.
e) Salts formation, soaps, detergentes and tensoactives.
f) Esterification reactions.
g) Acylhalides formation, anhydrides, esters and amides.
h) Carboxylic group reduction.

12. Carboxylic acid derivatives: esters, amides, acylhalides, carboxylic acid anhydrides.
a) Structure and properties.
b) Occurrence and use.
c) Description by the Valence and Orbital Molecular theories.
d) General mechanism of the nucleophile additions to carboxylic acid and derivatives.
f) Hydrolysis reaction.
g) Possible interconversion reactions of derivatives.
h) Acidity of the hydrogen in α position of carboxylic acids and derivatives.
i) Enolates formation, alkylation reactions and aldolic condensation.
j) Addition of organometallic reagentes 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 and Orbital Molecular theories.
e) The Hückel rule.
f) Lateral chain reactions of aromatic compounds: S_N2, S_N1, hydrogenolysis, oxidation.
g) Birch reduction.

14. Aromatic electrophilic substitution reactions
a) Reactions of halogenation, nitration, sulphonation, Friedel-Crafts alkylation and acylation.
b) Orientation effects in Ar_ES.
c) Effects of multiple substituents

15. Amines
a) Structure and properties.
b) Sources and uses.
c) Basicity and salts formation.
d) Imines and enamines formation.
e) Preparation methods: alkylation, reduction of nitro-compounds, nitriles, azides, imines and oximes.
f) Reductive amination.
g) Hofman and Curtius rearrangements.
h) Diazonium salts formation.

16. Heterocyclic compounds: examples, properties and some syntheses.

Bibliography

a) Solomons, G.; Fryhle, C. "Organic Chemistry", 8th ed., 2004; John Wiley & Sons Inc.: NY;

b) Streitweiser, A.; Heathcook, C.H.; Kosower, E.M. "Introduction to Organic Chemistry", 4th ed., 1992; MacMillan Publis. Comp.: NY;

c) Clayden, J.; Greeves, N.; Warren, S.; Wothers, P. "Organic Chemistry", 2004; Oxford Univ. Press: Oxford;

d) Carey, F. A. "Organic Chemistry", 5th ed., 2003; McGraw-Hill, Inc.: NY.
a) Solomons, G.; Fryhle, C. "Organic Chemistry", 8th ed., 2004; John Wiley & Sons Inc.: NY;
b) Streitweiser, A.; Heathcook, C.H.; Kosower, E.M. "Introduction to Organic Chemistry", 4th ed., 1992; MacMillan Publis. Comp.: NY;
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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.