Code: QO321

Name: Química orgânica I

Name in English: Organic Chemistry I

Name in Spanish: Química Orgánica I

Subject type: Organic Chemistry

Approval Type: Grade and Frequency

Characteristic: Regular

Frequency: 75%

Period Type / Offering period: Semiannual/All periods

Requires Final Exam: Yes

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
4						**4**	**15**	**4**

Occurrence on curriculum: 05, 50, 56, 63

Pre requirement: QG101 + QG102 or 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:

1. Introduction to the discipline:
Organic chemistry as 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;
g) Molecular geometry.

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

4. Introduction to organic reactions. Acidity and basicity
a) Examples of organic reactions, equilibrium.
b) Acid-base reactions, Bronsted and Lewis acids and bases;
c) The strength of acids and bases, Ka and pKa;
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 dissociationenergy;
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: heatsof hydrogenation
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. 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.

Basic Bibliography

1) MCMURRY, J. "**Organic chemistry**", 9a Edition, Cengage Learning, Nova Iorque, 2015. ISBN: 978-1305080-485

2) LOUDON, M. e PARISE, J. "**Organic chemistry**", 7a Edition, W. H. Freeman, Nova Iorque, 2021. ISBN: 978-1-319188-429

3) WADE, L. e SIMEK, J. W. "**Organic chemistry**", 9a Edition, Pearson Education, Minneapolis, 2016. ISBN: 978-0-321971-371

Supplementary Bibliography

1) CLAYDEN, J.; GREEVES, N. E WARREN, S. "**Organic chemistry**", 2a Edition, Oxford University Press, Florença, 2012. ISBN: 978-0-199270-293

2) MCMURRY, J. E. e BEGLEY, T. P. "**Organic chemistry of biological pathways**", 2a edição, W. H. Freeman, Pacific Groove, 2015, ISBN: 978-1-936221-561

3) ARPE, H. J. "**Industrial organic chemistry**", 5a Edition, Wiley, New Jersey, 2010. ISBN: 978-3-52732002-8

4) KLEIN, D. "**Organic chemistry**", 4a edition, Wiley, New Jersey, 2020. ISBN: 978-1-119659-594

5) BROWN, W. H.; IVERSON, B. L.; ANSLYN, E. E FOOTE, C. S. "**Organic chemistry**", 9a edition, Cengage Learning, Nova Iorque, 2022. ISBN: 978-0-357451-861