Code: QO858

Name: Introdução à Físico-Química Orgânica

Name in English: Introduction to Physical Organic Chemistry

Name in Spanish: Introducción a la Química Física Orgánica

Subject type: Weekly

Approval Type: Grade and attendance

Characteristic: Regular

Frequency: 75%

Period Type / Offering period: Semester-based / As determined by the Teaching Unit

Requires Final Exam: Yes

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
2	**0**	**0**	**0**	**0**	**00**	**2**	**15**	**30**

Occurrence on curriculum: Second semester

Pre requirement: QO521 or QO327 or QO427 or QO421

Summary: Structure and chemical bond models, Thermodynamics and stability of organic compounds, Conformational and stereochemical analysis, Potential energy surfaces and kinetic analysis of organic reactions, Tools for studying reaction mechanisms and their applications in addition and elimination reactions, substitution reactions and rearrangements; Introduction to theoretical calculations to understand the structure and reactivity of organic compounds.

Program:

1. Structure and chemical bond models

2. Thermodynamics and stability of organic compounds

a) Enthalpy, entropy and Gibbs free energy

b) Thermodynamics of stable organic compounds and reactive intermediates

3. Conformational analysis

a) Steric, electrostatic and stereoelectronic effects

b) Spectroscopic methods in conformational analysis

4. Potential energy surfaces and kinetic analysis of organic reactions

a) Transition state theory

b) Postulates and principles related to reaction kinetics

c) Kinetic analysis for simple mechanisms

5. Tools related to reaction mechanism studies

a) Kinetic isotopic effects

b) Linear free energy relationships

c) Experiments to study reaction mechanisms

6. Applications in addition, substitution and rearrangement reactions

7. Introduction to theoretical calculations to understand the structure and reactivity of organic compounds.

a) Computational chemistry methods

b) Calculations of structural and spectroscopic properties

c) Natural Bond Orbitals (NBO)

d) Quantum theory of atoms in molecules (QTAIM)

Basic Bibliography

1) ANSLYN, E. V.; DOUGHERTY, D. A. **Modern physical organic chemistry**. University Science: California, 2006.
2) CARROLL, F. A. **Perspectives on Structure and Mechanism in Organic Chemistry**. 2nd Ed., Wiley, New Jersey, 2011.
3) FLEMING, I. **Molecular Orbitals and Organic Chemical Reactions**

Supplementary Bibliography

1) ALABUGIN, I**.** ***Stereoelectronic Effects: A Bridge Between Structure and Reactivity***, John Wiley & Sons, 2016.
2) GROSSMAN, R. ***The Art of Writing Reasonable Organic Reaction Mechanisms***, Springer, 2019.
3) CAREY, F.; SUNDBERG, R. ***Advanced Organic Chemistry: Part A: Structure and Mechanisms****,* 5a ed., Springer, 2006.
4) HEHRE, W. J.; SHUSTERMAN, A. J.; NELSON, J. E. ***The Molecular Modelling Workbook for Organic Chemistry***, 6th Ed., Prentice Hall, 2005.
5) CLAYDEN, J.; GREEVES, N.; WARREN, S. ***Organic Chemistry***, 2a Ed., Oxford University Press, USA 2012.