UNIVERSIDADE ESTADUAL DE CAMPINAS
INSTITUTO DE QUÍMICA

PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	**Name**
QO858	Introduction to Physical Organic Chemistry

Vector
OF:S-6 T:002 P:000 L:000 O:000 D:000 HS:002 SL:002 C:002 AV:N EX:S FM:75%

Pre requirement	QO521

Summary

Structure and models of chemical bonding, Thermodynamics and stability of organic compounds, Structure and stereochemistry analysis, Potential energy surfaces and kinetic analysis of organic reactions, and rearrangements; Introduction to theoretical calculations for understanding the structure and reactivity of organic compounds.

Program

1. Structure and chemical bonding 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 of study of reaction mechanisms
a) Kinetic isotopic effects
b) Linear free energy relationships
c) Experiments related to the study of reaction mechanisms
6. Applications in addition, substitution and rearrangement reactions
7. Introduction to theoretical calculations for understanding the structure and reactivity of organic compounds.
a) Methods of computational chemistry
b) Calculations of structural and spectroscopic properties
c) Natural Bond Orbitals (NBO)
d) Quantum theory of atoms in molecules (QTAIM)

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.

Evaluation criteria

Evaluation criteria defined by the Professor, based on the provisions of Section I - General norms, Chapter V - Student Assessment in Discipline, of the General Undergraduate Regiment. Frequency: 75% (* The absences will be considered within the provisions of chapter VI, section X, article 72 of the General Undergraduate Regulations)