CH-431

# Physical and computational organic chemistry

Corminboeuf Clémence

| Cursus | Sem. | Type |
|---|---|---|
| Chimiste | MA2 | Opt. |

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|---|---|
| Language of teaching | English |
| Credits | 2 |
| Session | Summer |
| Semester | Spring |
| Exam | Oral |
| Workload | 60h |
| Weeks | 14 |
| **Hours** | **2 weekly** |
| Courses | 2 weekly |
| **Number of positions** | |

## Summary

This course introduces computational electronic structure methods and their broad applications to organic chemistry. It also discusses physical organic concepts to illustrate the stability and reactivity of organic molecules.

## Content

**Computational Methods**

- Electronic structure approaches for organic chemistry
- Overview of density functional theory and post-Hartree-Fock methods

**Fundamentals of physical organic chemistry**

- Thermodynamic stabilities
- Stabilizing effects
- Computation of reaction mechanisms
- Radicals, diradicals, carbenes and spin multiplicity
- Kinetic isotope effects
- (Organic reactions dynamics)

**Special topic in physical organic chemistry**

- Aromaticity
- Carbocation
- Molecular Strain

**Selected article for presentation**

## Keywords

Computational organic chemistry, chemical concepts

## Learning Outcomes

By the end of the course, the student must be able to:

- Choose an appropriate computational method to address a given chemistry problem
- Estimate the uncertainties associated with the use of a given computational approach
- Assess / Evaluate the (de)stabilizing effects of a molecule
- Elaborate orbital energy diagrammes

- Interpret the forbidden/allowed nature of a chemical reaction
- Specify the type of kinetic isotope effects
- Identify the main message of an article

### Transversal skills

- Communicate effectively, being understood, including across different languages and cultures.

### Expected student activities

resolve the weekly mini-quiz and the two maxi-quiz
read, understand and present a scientific article

### Assessment methods

1/3 présentation; 2/3 oral exam

### Resources

#### Ressources en bibliothèque

- Computational Organic Chemistry / Bachrach
- Modern Physical Organic Chemistry / Anslyn

#### Websites

- http://scgc.epfl.ch/telechargement_cours_chimie

#### Moodle Link

- http://moodle.epfl.ch/course/view.php?id=15018