

212045 – COMPUTATIONAL METHODS OF ANALYSIS

CREDITS: 04 (four) – 60 hours/class

CONTENT:

Molecular structure; Infrared and Raman spectroscopy; NMR spectroscopy; UV/Vis spectroscopy; Mechanisms of organic and inorganic reactions; Solvent effect.

SYLLABUS:

1. Introduction to computational chemistry and its potentialities;
2. Representation of the structure in molecular coordinates;
3. Stable molecular structure prediction - Geometry optimization;
4. Obtaining and visualizing molecular orbitals;
5. Vibrational spectroscopy (obtaining and interpreting infrared and Raman spectra);
6. Obtaining thermochemical properties;
7. Electron spectroscopy (obtaining and interpreting UV / Vis spectra);
8. Nuclear Magnetic Resonance Spectroscopy (obtaining and interpreting ^1H NMR, ^{13}C , ^{195}Pt , etc. spectra);
9. Studies of mechanisms from organic and inorganic reactions;
10. Prediction of the effect from the solvent on the structure, properties and reactivity of molecules.

BIBLIOGRAPHY:

1. CRAMER, Christopher J. Essentials of Computational Chemistry: theories and models. John Wiley & Sons, 2009.
2. HEINE, Thomas; JOSWIG, Jan-Ole; GELESSUS, Achim. Computational Chemistry Workbook: learning through examples. Wiley-VCH, 2009.
3. HINCHLIFFE, Alan. Molecular Modelling for Beginners. John Wiley & Sons, 2003.
4. YOUNG, David. Computational Chemistry: a practical guide for applying techniques to real world problems. John Wiley & Sons, 2001.
5. Scientific articles.