Course Syllabus

Department/Faculty
School of Engineering

Graduate Program
Materials Engineering and Nanotechnology

Degree
☒ Academic Master's ☒ Doctorate (PhD) ☐ Professional Master's

Course Name
Advanced Spectroscopic Methods

Professor(s)

Office hours
48

Course Overview

The discipline deals with the study of the theoretical foundations and applications of spectroscopic and spectrometric techniques. The techniques covered are the following: infrared spectroscopy, Raman spectroscopy, X-ray excited photoelectron spectroscopy, UV-Vis spectroscopy and mass spectrometry.

Campus Higienópolis: *Rua da Consolação, 896 – Edifício João Calvino - 8º andar ● Consolação ● São Paulo - SP ● CEP 01302-907*
Tel. (11) 2114-8143 ● **www.mackenzie.br** ● **prpg.cgpos@mackenzie.br**

Program content:

1 - Infrared Spectroscopy:

Principles of the technique. Fourier transform. Sample preparation procedures. Spectra interpretation. Practical applications.

2 - Raman Spectroscopy:

Principles of the method. Sample preparation procedures. Spectra interpretation. Practical applications.

3 - X-ray excited photoelectron spectroscopy:

Determination of binding energies in solids and liquids, study of surfaces, identification of elements, instrumentation, sample handling, spectra interpretation, areas of application.

4 - UV-Vis Spectroscopy:

Fundamentals of technique; relationship between absorption and concentration: Lambert-Beer law; absorption spectra; spectrophotometric instrumentation; deviations from the Lambert-Beer Law. Practical applications.

5- Mass spectrometry:

Fundaments of the technique: nominal and exact masses (molecular formula), rules (nitrogen, Stevenson), resolution, isotopic patterns, molecular ions and main fragmentation routes, and ion detection.

Principles and applications of the main ionization techniques: EI, ESI, MALDI, APCI, APPI and ambient ionization techniques: DESI, DART, EASI.

Principles and applications of the main mass analyzers: quadrupoles, ion traps, TOFs and orbitraps.

Uses of the technique in applied chemistry as in omic sciences, forensics, new materials, natural products, fuels, and food chemistry.

Letter Grade Assignment
Grade A (Excellent) - Grade points between 9 and 10
Grade B (Good) - Grade points between 8 and 8.9
Grade C (Satisfactory) - Grade points between 7 and 7.9
Grade D (Unsatisfactory) - Grade points between 0 and 6.9

Campus Higienópolis: *Rua da Consolação, 896 – Edifício João Calvino - 8º andar ● Consolação ● São Paulo - SP ● CEP 01302-907*
Tel. (11) 2114-8143 ● **www.mackenzie.br** ● **prpg.cgpos@mackenzie.br**

Texts, Materials, and supplies

Basic Bibliography

DOMIN, M.; CODY, R. **Ambient Ionization Mass Spectrometry (New Developments in Mass Spectrometry)**. 1st Edition, Royal Society of Chemistry, 2015.

McHALE, J.L.. **Molecular Spectroscopy.** CRC Press; 2017.

LAMBERT, J.B.; MAZZOLA, E.B.; RIDGE,C.D. **Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications, and Experimental Methods**. UK, Wiley, 2019

SKOOG, D. A.; HOLLER, F. J., NIEMAN, T. A., **Princípios de Análise Instrumental**, 6ª edição, Bookman: São Paulo, 2009.

Bibliografia Complementar

WATSON, J. THROCK; SPARKMAN, O. DAVID. **Introduction to Mass Spectrometry: Instrumentation, Applications, and Strategies for Data Interpretation**, UK, Wiley 2007.
Artigos científicos recentes.

SALA, O. **Fundamentos da Espectroscopia Raman e no Infravermelho** - 2ª Edição, Editora UNESP, 2008.

HOFFMANN, EDMOND; STROOBANT, VINCENT. **Mass Spectrometry: Principles and Applications**, 3rd EditioN, UK, Wiley 2007.

WATTS, JOHN F.; WOLSTENHOLME, JOHN. **An introduction to surface analysis by XPS and AES. UK,** Wiley 2009**.**