



UNIVERSIDADE PRESBITERIANA MACKENZIE

Pró-Reitoria de Pesquisa e Pós-Graduação
Coordenadoria Geral de Pós-Graduação Stricto Sensu



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 Prof. Dr. Marcos Nogueira Eberlin		
Office hours 48		
Course Overview The course focuses on the study of the theoretical foundations and applications of spectroscopic and spectrometric techniques. The topics covered include: infrared spectroscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, UV-Vis spectroscopy, and mass spectrometry.		



Topics outline

1 – Infrared Spectroscopy:

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

2 – Raman Spectroscopy:

Method principles. Sample preparation procedures. Spectrum interpretation. Practical applications.

3 – X-ray Photoelectron Spectroscopy (XPS):

Determination of binding energies in solids and liquids, surface studies, element identification, instrumentation, sample handling, spectrum interpretation, and application areas.

4 – UV-Vis Spectroscopy:

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

5 – Mass Spectrometry:

Fundamentals of the technique: nominal and exact masses (molecular formula), rules (nitrogen rule, Stevenson's rule), resolution, isotopic patterns, molecular ions and major fragmentations, and detection.

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

Principles and applications of the main mass analysers: quadrupoles, ion traps, TOFs, and Orbitraps.

Application of the technique in applied chemistry, such as in ohmic sciences, forensics, new materials, natural products, fuels, and food.

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



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. *Principles of Instrumental Analysis*, 6th edition, Bookman: São Paulo, 2009.

Additional Bibliography

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

Recent scientific articles.

SALA, O. *Fundamentals of Raman and Infrared Spectroscopy*, 2nd Edition, 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.