



UNIVERSITÀ DEGLI STUDI DI PALERMO

DEPARTMENT	Fisica e Chimica - Emilio Segrè
ACADEMIC YEAR	2018/2019
MASTER'S DEGREE (MSC)	CHEMISTRY
SUBJECT	ORGANIC SPECTROSCOPY
TYPE OF EDUCATIONAL ACTIVITY	B
AMBIT	50485-Discipline chimiche organiche
CODE	19814
SCIENTIFIC SECTOR(S)	CHIM/06
HEAD PROFESSOR(S)	LO MEO PAOLO MARIA Professore Associato Univ. di PALERMO GIUSEPPE
OTHER PROFESSOR(S)	
CREDITS	6
INDIVIDUAL STUDY (Hrs)	98
COURSE ACTIVITY (Hrs)	52
PROPAEDEUTICAL SUBJECTS	
MUTUALIZATION	
YEAR	1
TERM (SEMESTER)	1° semester
ATTENDANCE	Mandatory
EVALUATION	Out of 30
TEACHER OFFICE HOURS	LO MEO PAOLO MARIA GIUSEPPE Monday 15:00 17:00 Studio del docente, V.le delle Scienze Ed. 17.

DOCENTE: Prof. PAOLO MARIA GIUSEPPE LO MEO

PREREQUISITES	Basic knowledge of Organic Chemistry and Physical Chemistry, principles of quantum mechanics, matter-electromagnetic wave interaction and basics of UV-Vis spectroscopy, electric and magnetic field and their interaction with charged particles.
LEARNING OUTCOMES	<p>Knowledge and understanding: Knowing the main spectroscopic techniques used to study organic molecules and their aggregates. Ability to use the specific language of the discipline.</p> <p>Applying knowledge and understanding: Ability to recognize and organize independently, the general principles of the discipline in the data discussion and interpretation of data concerning organic structures. Ability to apply the most common spectroscopic techniques to solve problems concerning organic and supramolecular structures.</p> <p>Making judgments: Be able to reasonably predict the spectroscopic response of an organic structure.</p> <p>Communication skills: Ability to expose, even to a non-expert audience, the results of spectroscopic elucidation of an organic structure.</p> <p>Learning ability: Ability to upgrade one's own knowledge of the discipline by consultation of relevant field literature.</p>
ASSESSMENT METHODS	<p>The exam consists in: a) a written test (90 minutes) concerning the interpretation of the spectra of an organic molecule; b) an oral discussion concerning the topics of the course (at least three questions).</p> <p>The final evaluation will be graded taking into consideration:</p> <p>a) Basic knowledge of the concepts and limited ability of analysis of the cases discussed during the examination (18-21 rating); b) Good knowledge of the concepts and fair capacity of applying them to the cases proposed during the examination (22-25 rating); c) In-depth knowledge of the theory and skills to apply to cases proposed, albeit in a not completely independent way (26-28 rating); d) In-depth knowledge of the theory, ability to apply it promptly and properly to the proposed cases, ability to formulate interdisciplinary links, excellent property of expression (29-30L rating).</p>
EDUCATIONAL OBJECTIVES	The Organic Spectroscopy course aims to provide and improve the necessary know-how on the use of modern physical and spectrometric methods for the elucidation of structural problems concerning organic molecules and supramolecular aggregates
TEACHING METHODS	Front lectures and exercises.
SUGGESTED BIBLIOGRAPHY	<ul style="list-style-type: none"> - Silverstein et al., Identificazione spettrometrica di composti organici, CEA (2a ed. 2006) - Hesse et al. Metodi Spettroscopici in Chimica Organica, Edisies (2a ed. 2010) - de Hoffmann, Stroobant, Mass Spectrometry principles and applications, WILEY (3a ed. 2007) - dispense fornite dal docente.

SYLLABUS

Hrs	Frontal teaching
2	Generalities in spectroscopy: wave-matter interaction and its consequences; the general problem of structure elucidation in organic and supramolecular chemistry, basics of UV-vis spectroscopy.
3	IR spectroscopy: generalities, recognition of functional groups by IR spectroscopy, factors affecting the vibration frequencies of main functional groups, FT-IR techniques.
3	Mass-spectrometry methods: the "classic" technique by electron impact and magnetic analysis, and related problems; QET and its consequences, fragmentation in EI-MS, fragmentation patterns of main classes of organic molecules; resolution in MS and related problems.
2	Other ionization methods in MS: CI, FAB, MALDI, ESI and their applications
3	Other analyzers in MS: electrostatic analyzer and its coupling with the magnetic analyzer; quadrupole analyzer and ionic trap, TOF, ICR, hybrid analyzers (Q-TOF), Orbitrap.
4	MS-MS techniques and their main uses. Applications of mass spectrometry to the study of biomolecules (proteins, fats) and supramolecular systems.
3	Introduction to Nuclear Magnetic Resonance spectroscopy: nuclear spin theory, excitation of nuclei having spin $\frac{1}{2}$, concept of chemical shift; the "classic" CW-NMR technique; ^1H -NMR spectroscopy: structural factors affecting ^1H chemical shift, magnetic anisotropy of unsaturated groups and its consequences.
4	General theory of pulse NMR: magnetization, pulse, its characteristics and interaction with the sample, nuclear relaxation, FID and its treatment, concepts of channel and pulse sequence; relaxation times and their determination ("inversion-recovery" and "spin-echo").
5	Theory of spin-spin coupling: signal multiplicity; coupling constant and factors affecting its value, Karplus rule; double irradiation techniques: selective decoupling and polarization transfer; Nuclear Overhauser Effect (NOE) and its application to stereochemistry problems; multiple spin systems; chemical shift equivalence and magnetic equivalence in relation to molecular symmetry.

SYLLABUS

Hrs	Frontal teaching
3	¹³ C-NMR spectroscopy: generalities, factors affecting ¹³ C chemical shift; ¹ H- ¹³ C decoupling and its consequences, gated decoupling and inverse-gated decoupling, polarization transfer and the sequence INEPT, DEPT.
6	2D-NMR techniques: homo- and hetero-correlation, COSY, HETCOR, HMQC, HSQC, COLOC and HMBC spectra, ¹³ C- ¹³ C correlation, INADEQUATE spectra; 1D- and 2D-TOCSY techniques, HMQC-TOCSY; NOESY and ROESY techniques; applications of 2D-NMR to biomolecules and supramolecular systems.
2	Particular applications of NMR spectroscopy: dynamic NMR and its applications; Solid-state NMR.
Hrs	Practice
12	Combined interpretation of spectra (IR, MS, 1D and 2D NMR) of organic molecules and biomolecules.