UNIVERSITÀ DEGLI STUDI DI PALERMO

DEPARTMENT	Fisica e Chimica - Emilio Segrè
ACADEMIC YEAR	2020/2021
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 ans basics of UV-Vis spectroscopy, electric and magnetic field and their interaction with charged particles.
LEARNING OUTCOMES	Knowledge and understanding: Knowing the main modern spectroscopic techniques used to study organic molecules, their aggregates, and organic materials. Ability to use the specific language of the discipline. 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 (molecular, macromolecular and supramolecular) structures. Ability to apply the most common spectroscopic techniques to solve problems concerning organic structures. Making judgments: Be able to reasonably predict the spectroscopic response of an organic structure. Communication skills: Ability to expose, even to a non-expert audience, the results of spectroscopic elucidation of an organic structure. Learning ability: Ability to upgrade one's own knowledge of the discipline by consultation of relevant field literature.
ASSESSMENT METHODS	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). On the whole, the exam is aimed at evaluating the acquisition of the discipline concepts, Moreover, favourable appreciation will be granted to the abilities of: i) correctly and confidently using the peculiar discipline language; ii) catching crosslinks with all the aspects of modern organic chemistry (including supramolecular and materials chemistry); iii) elaborating information relevant to a study case, in such a way to rationalize the observed behavior and forsee new observations. Ranking will be marked in thirtieths. The final evaluation will be graded considering: 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 ability of applying them to the cases proposed during the examination, though in a not completely autonomous way (22-25 rating); c) Excellent knowledge of the theory and ability to apply it to cases proposed (26-28 rating); d) Very in-depth knowledge of the theory, ability to apply it promptly and properly to the proposed cases, ability to formulate interdisciplinary crosslinks (particularly with supramolecular and materials chemistry), excellent expression skills (29-30L rating).
EDUCATIONAL OBJECTIVES	The Organic Spectroscopy course aims at providing and improving the necessary know-how on the use of modern physical and spectrometric methods for the elucidation of problems concerning organic molecular structures, including supramolecular aggregates, biomolecules and organic materials.
TEACHING METHODS	Front lectures and exercises.
SUGGESTED BIBLIOGRAPHY	- 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) - Friebolin, Basic One- and Two-Dimensional NMR Spectroscopy, WILEY (5a ed. 2010).

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.
4	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
2	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.

SYLLABUS

Hrs	Frontal teaching
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 ½, 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 affectng 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.
3	13C-NMR spectroscopy: generalities, factors affecting 13C chemical shift; 1H-13C decoupling and its consequences, inverse-gated decoupling, polarization transfer and the sequence INEPT, DEPT.
5	2D-NMR techniques: homo- and hetero-correlation, COSY, HETCOR, HMQC, HSQC, COLOC and HMBC spectra, 13C-13C correlation, INADEQUATE spectra; 1D- and 2D-TOCSY techniques, HMQC-TOCSY; NOESY and ROESY techniques; applications of 2D-NMR to biomolecules and supramolecular systems.
3	Particular applications of NMR spectroscopy: dynamic NMR and its applications; Solid-state NMR, FFC-NMR.

Hrs	Practice
12	Combined interpretation of spectra (IR, MS, 1D and 2D NMR) of organic molecules and biomolecules.