UNIVERSITÀ DEGLI STUDI DI PALERMO

DEPARTMENT	Fisica e Chimica - Emilio Segrè
ACADEMIC YEAR	2016/2017
MASTER'S DEGREE (MSC)	CHEMISTRY
INTEGRATED COURSE	SUPRAMOLECULAR CHEMISTRY WITH SPECTROSCOPY APPLICATIONS
CODE	16493
MODULES	Yes
NUMBER OF MODULES	2
SCIENTIFIC SECTOR(S)	CHIM/06
HEAD PROFESSOR(S)	
OTHER PROFESSOR(S)	NOTO RENATO — Cultore della Materia — Univ. di PALERMO LO MEO PAOLO MARIA GIUSEPPE — Professore Associato — Univ. di PALERMO
CREDITS	12
PROPAEDEUTICAL SUBJECTS	
MUTUALIZATION	
YEAR	1
TERM (SEMESTER)	2° semester
ATTENDANCE	Not 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. **NOTO RENATO** Monday 11:00 13:00 studio docente Friday 11:00 13:00 studio docente

DOCENTE:

PREREQUISITES	Basic knowledge of Organic Chemistry and Inorganic Chemistry, chemical thermodynamics and kinetics, principles of quantum mechanics, electric and magnetic field and their interaction with charged particles.
LEARNING OUTCOMES	Knowledge and understanding Know the main weak interactions between molecular entities. Knowing the basics involving good molecular recognition properties by a host. Knowing the most common supramolecular systems. Know the main spectroscopic techniques in reference to supramolecular systems. Acquisition of the tools for the preparation of a study of intermolecular interactions. Ability to use your own specific language of this discipline. Applying knowledge and understanding Ability to recognize and organize independently, the general principles of the discipline in the data discussion and interpretation regarding supramolecular structures. Ability to apply the most common spectroscopic techniques to solve problems concerning the weak interactions between molecules. Making judgments Be able to assess when they are potential weak interactions between molecules and bring, as appropriate, experimental results to the basic principles of the discipline. communication skills Ability to expose, even to a non-expert audience, the results of different studies organized systems and bring them back to the basic principles of the discipline. Learning ability ability to upgrade and expansion of knowledge on discipline through consultation with its scientific publications in the field
ASSESSMENT METHODS	The exam consists of: a) a written test (90 minutes) concerning the interpretation of the spectra of an organic molecule; b) an oral discussion concerning the subjects of both modules (at least four questions). The exam overall aims at evaluating the acquisition of the contents of the single modules. Moreover, positive marks will reward the ability to use correctly the specific disciplinary language, the ability to make interdisciplinary connections with all the aspects of modern organic chemistry, and the ability to elaborate information concerning a study system in order to rationalize its behavior and forecast new observations. Final marks are expressed as out of 30.
TEACHING METHODS	Lessons, exercises

MODULE
SPECTROSCOPIC METHODS IN ORGANIC AND SUPRAMOLECULAR CHEMISTRY

Prof. PAOLO MARIA GIUSEPPE LO MEO

SUGGESTED BIBLIOGRAPHY

- Silverstein et al., Identificazione spettroscopica di composti organici, CEA
- Pedulli, Metodi fisici in chimica organica, Piccin.
- Skoog-Leary, Chimica Analitica Strmentale, Edises.
- de Hoffmann, Stroobant, Mass Spectrometry principles and applications, WILEY
- dispense fornite dal docente.

AMBIT	50485-Discipline chimiche organiche
INDIVIDUAL STUDY (Hrs)	95
COURSE ACTIVITY (Hrs)	55

EDUCATIONAL OBJECTIVES OF THE MODULE

The Spectroscopic Methodologies in Organic and Supramolecular Chemistry 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.

SYLLABUS

Hrs	Frontal teaching
3	Generalities in spectroscopy: wave-matter interaction and its consequences; the genertal 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 "classical" 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
3	Other ionization methods in MS: CI, FAB, MALDI, ESI and their applications.
3	MS analyzers: electrostatic analyzer and its coupling with magnetic analyzers; quadrupole analyzer and ionic trap, TOF, ICR.
4	MS-MS techniques and their main uses. Applications of mass spectrometry to the study of biomolecules (proteins, fats) and supramolecular systems.
6	Introduction to Nuclear Magnetic Resonance spectroscopy: nuclear spin theory, excitations of nuclei having spin ½, concept of chemical shift; the "classic CW-NMR technique; 1H.NMR spectroscopy: structural factosr affecting 1H chemical shift, magnetic anisotropy of unsaturated groups and its consequences. Theory of spin-spin coupling: signal multiplicity; coupling constants and factors affectng its value, Karplus rule; double irradiation techniques and selective decoupling; Nuclear Overhauser Effect (NOE) and its application to stereochemistry problems; multiple spin systems; chemical shift equivalence and magnetic equivalence in relation to molecular symmetry.
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.
3	13C-NMR spectroscopy: generalities, factors affecting 13C chemical shift; 1H-13C decoupling and its consequences, gated decoupling and inverse-gated decoupling, polarization transfert and the sequence INEPT, DEPT.
6	2D-NMR techniques: homo- and hetero-correlation, COSY, HETCOR, HMQC, HSQC, COLOC and HMBC spectra, 13C-13C correlation, INADEQUATE; 1D- and 2D-TOCSY techniques, HMQC-TOCSY, NOESY and ROESY techniques; applications of 2D-NMR to biomolecules and supramolecular systems.
2	Dynamic NMR and solid-state NMR techniques and their applications.

Hrs	Workshops
15	Combined interpretation of MS, IR and NMR (1D and 2D) spectra.

MODULE
SUPRAMOLECULAR CHEMISTRY

Prof. RENATO NOTO

SUGGESTED BIBLIOGRAPHY	
-J. W. Steed, J. L. Atwood “Supramolecular Chemistry” Wiley. -Fotocopie di articoli e/o review fornite dal docente	
AMBIT	50485-Discipline chimiche organiche
INDIVIDUAL STUDY (Hrs)	102
COURSE ACTIVITY (Hrs)	48
EDUCATIONAL OBJECTIVES OF THE MODULE	
The course of Supramolecular Chemistry aims to develop knowledge about the weak interactions between molecular entities and the consequences related to these interactions both in the field of Life Sciences and in the field of Materials Chemistry.	

SYLLABUS

Hrs	Frontal teaching
1	Brief History of the Supramolecular Chemistry
3	Clathrates and cavitated
6	intramolecular forces, selectivity, chelating effect, macrocycle effect, pre-planning and complementarity.
10	Crown ethers: general information on synthesis, nomenclature, structure, complexing properties. Calixarenes: general information on synthesis, nomenclature, conformational equilibria, complexing capacity. Lariat ethers, podands, spherands.
4	Receptors for anions. Comparison between the recognition of cations and anions. Katapinandi, tetrahedral receptors, linear receptors.
5	Receptors for neutral molecules. Cyclodextrins: functionalization, complexing properties.
5	Zeolites, clathrates and hydrate clathrates.
10	Ionic liquids: nomenclature, structure, properties, catalytic effects. LCD. Gel: characteristics, structure and properties.
4	Nanochemistry, molecular machines, nanotubes, fullerenes