LOGO DELLA STRUTTURA PRIMARIA

COURSE: Spectroscopic Methods in Organic Chemistry			
ACADEMIC YEAR:2016-2017			
TYPE OF EDUCATIONAL ACTIVITY: Basic			
TEACHER: Prof. Antonietta Pepe			
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Language: Italian (English on request)			
ECTS: 6 (6 of lessons)	n. of hours: 48 (48 of lessons)	Campus: Potenza/Matera Dept./School: Department of Science Program:Chemistry (L27)	Semester: I

EDUCATIONAL GOALS AND EXPECTED LEARNING OUTCOMES

The aim of the course is to provide a theoretical and practical knowledge on spectroscopic methods so that the students could perform the structural characterization of an unknown organic compound using in a combined way the spectroscopic techniques: IR, MS and NMR, which are routinely used in a chemistry laboratory, also at the industrial level. All students will be trained in interpreting individual spectra and sets of spectra obtained by different methods, so that molecular compounds and materials are quickly and efficiently characterized with respect to their structure and stereochemistry. Special emphasis will be placed on discussing, documenting and reporting the data.

After having completed the course, the student should:

1) Understand principles of all of the above mentioned spectroscopic methods.
2) Be able to extract specific information about structure of a compound from various spectra.
3) Be skilled enough to elucidate an unknown structure, or solve a structure-related problem, by combining information obtained from various spectroscopic methods.
4) Be able to choose spectroscopic methods which are the most suitable for a given problem.
5) be able to report spectral data of organic molecules, following the common guidelines of Organic Chemistry Journals.

PRE-REQUIREMENTS

In order to understand the basis of the spectroscopic techniques and the main applications in Organic Chemistry, the student should have good knowledge of the basic principles of General, Inorganic and Organic Chemistry, of Physics and Physical Chemistry.

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SYLLABUS

General introduction to the structural determination of organic molecules (1h)

Mass Spectrometry (8h). Block diagram of the spectrometer. Generation of ions by electronic impact (EI). Exact mass and molecular formula. Molecular ion and the distribution of isotopic peaks. Primary and secondary fragmentations. Principal rules of fragmentation and their application to the most common classes of organic compounds.

Energy of the radiations in the electromagnetic spectrum and their spectroscopic techniques (1h).

NMR spectroscopy (6h).Magnetic features of the nuclei and the resonance conditions for 1H,13C and other nuclei. The rotating frame model, the concept of magnetization, conditions of on and off resonance and definition of spectral window. Concept of selective and hard pulse, 90° and 180° pulses and their effects on the magnetization. Block diagram of the NMR spectrometer, signal acquisition and some references on the FT and the signal processing.

^{1}H NMR (8h). Definition of chemical shift and coupling constants. The Karplus equation. Spectral multiplicity, chemical and magnetic equivalence. Strength of the magnetic field and spin systems of 1st and 2nd order: AX, AB, AMX, ABX and AA'XX'. Homo and heteronuclear selective decoupling, broadband decoupling (WALTZ). T1 and T2 relaxation time mechanisms, and the effects on the signal. The nuclear Overhauser effect. Modulation of 1JCH, 1H-13C polarization transfer and the multipulse sequences INEPT and DEPT. Concept of two- dimensional NMR spectra. Bonds connectivity from chemical shift correlations in the COSY and HSQC experiments: with examples of 2D spectra interpretation.

^{13}C NMR (4h). Sensitivity. Proton decoupling and Noe effect. Factors defining the intensity of the signals. Factors defining the chemical shift. Additivity rules. DEPT.

Brief introduction to Dynamic NMR and 2D NMR (4h).

IR spectroscopy (6h). Molecular vibrations and the approximation group. Characteristic absorptions of the most common functional groups. Practical features of the IR spectroscopy. Exercises of structural determination of unknown structures are solved in the classroom by combining the treated spectroscopic techniques.

Exercises of increasing difficulties are proposed in the classroom on the interpretation of IR, MS, NMR spectra of unknown organic compounds (10h).

TEACHING METHODS

- Theoretical lessons with Classroom tutorials on combined analysis and interpretation of spectra of organic compounds in order to determine the molecular structure. Examples of exercises are proposed in the classroom with the active participation of student.
- Lectures of scientific papers published on organic chemistry journals, with particular emphasis on how the spectral data are reported.

EVALUATION METHODS

The aim of the final examination is to evaluate the level of achievement of the educational goals .

The final examination consists of two parts. A written examination (2h) where the student has to identify the molecular structure of an unknown organic compound by the combined analysis of IR, NMR and MS spectra and report the structural data using the common conventions of Organic Chemistry Journals. Once the written examination is approved, an Oral examination on the theoretical aspects of the spectroscopic and spectrometric techniques has to be taken.

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

- R.M. Silverstein, F.X. Webster, *Identificazione spettroscopica di composti organici*; Ambrosiana
- M. Hesse, H. Meier, B. Zeeh, *Metodi spettroscopici nella chimica organica*; EdiSES.
- Friebolin, *Basic One- and Two-Dimensional NMR Spectroscopy*, VCH;
- H. Gunther, *NMR Spectroscopy*; Wiley

Course slides will be available from a shared Dropbox folder, whose link will be furnished to the students attending the classroom. Furthermore, links to websites, where exercises are available, will be provided.

INTERACTION WITH STUDENTS

At the beginning of the course the teacher will describe the educational goals, the syllabus and the examination methods to the students and ask for the institutional emails of the attending students. All course information will be send to the provided email addresses.

Office hour: on monday and wednesday from 16.00 to 17.00; alternatively, by email appointment

EXAMINATION SESSIONS (FORECAST)

16/02/2017; 16/03/2017; 18/05/2017; 22/06/2017; 03/08/2017; 21/09/2017; 23/11/2017; 25/01/2018.

SEMINARS BY EXTERNAL EXPERTS YES □ NO □

FURTHER INFORMATION