NATIONAL UNIVERSITY OF ENGINEERING
COLLEGE OF SCIENCES
CHEMISTRY PROGRAM

CQ444 – ORGANIC CHEMISTRY IV

I. GENERAL INFORMATION

CODE	:	CQ444 – Organic Chemistry IV
SEMESTER	:	8
CREDITS	:	05
HOURS PER WEEK	:	07 (Theory – Practices)
PREREQUISITES	:	Organic Chemistry II
CONDITION	:	Mandatory

II. COURSE DESCRIPTION

Organic Chemistry IV is aimed at eighth-cycle students in the general formation area, being of a theoretical-practical nature. It provides the student with a complete introduction to the main spectroscopy techniques used for the elucidation of organic molecule structures: mass spectrometry, hydrogen and carbon nuclear magnetic resonance spectroscopy, infrared and ultraviolet spectroscopy. A problem solving approach is used through the interpretation of each of the spectra, masses and NMR in particular, with the support of the use of tables, identifying molecular fragments that allow to construct the global structure of the analyzed molecule.

III. COURSE OUTCOMES

By the end this course the student will:

- Identify the structural information provided by each spectroscopic technique.
- Recognize the advantages and disadvantages of the use of each of the techniques studied for a given molecule depending on its structure.
- Identify the skeletal structural elements provided by the MRI.
- Identify molecular peaks, presence of certain polyisotopic atoms and fragments and their applications to structural determination.
- Identify functional groups by means of IR spectroscopy.
- Identify chromophores and auxóchromes.
- Elucidate the total structure of an organic molecule from a series of spectra.

IV. LEARNING UNITS

1. **INTRODUCTION / 4 HOURS**
   Importance of spectroscopic techniques in the determination of organic structures (Mass Spectrometry, RMN1H, NMR13C, IR, and UV).

2. **MASS SPECTROMETRY / 8 HOURS**
   The mass spectrum / Fragmentation equations / Molecular ion and parent peak / Organic compounds (alkanes, alcohols, alkyl halides, ketones, etc.) and fragmentation equations / Spectrum interpretation.

3. **NUCLEAR MAGNETIC RESONANCE SPECTROMETRY OF HYDROGEN / 16 HOURS**
   The NMR^{1}H spectrum / Spectra characteristics. Signal origin: Nuclear spin. Chemical displacement and signals position / Protection and deprotection effects / (alkenes, alkynes, carbonyls and aromatics) / TMS. Delta scale / spin - spin coupling (Interaction between neighboring hydrogens) / JAB Coupling Constants / Spectra Interpretation / Vinyl systems. Analysis of problems involving mass spectra and RMN^{1}H.

4. **CARBON NUCLEAR MAGNETIC RESONANCE SPECTROMETRY / 18 HOURS**
   The NMR^{13}C spectrum / Spectrum characteristics / Chemical shift and position of the signals. Spectra classes / Spectrum interpretation.

5. **TWO-DIMENSIONAL MAGNETIC RESONANCE SPECTROSCOPY / 4 HOURS**
   Two-dimensional spectrum / Spectrum classes / Interpretation of spectra.

6. **INFRARED SPECTROSCOPY / 4 HOURS**
   IR spectrum / Spectrum characteristics / Signal origin / Absorption characteristics of the functional groups / Spectrum interpretation.

7. **ULTRAVIOLETE SPECTROSCOPY / 2 HOURS**
   UV spectrum / Spectrum characteristics / Signal origin / Absorption characteristics of the functional groups / Spectrum interpretation.

V. LABORATORIES AND PRACTICAL EXPERIENCES

Class practices (seminars). Since the 2nd week. Analysis and resolution of spectra, which are developed in parallel to the progress of the course.
Qualified practices (Total = four (04)). Each qualified practice consists of:

- Report (10 points). Development - at home (three problems). The syllabus will be given one week in advance.
- Written test (8 points), one hour long.
- Oral evaluation (2 points), which will be qualified with the participation of each student in the solution of the exercises proposed during the seminars and also during the classes.

VI. METHODOLOGY

The course is developed in theory sessions, class practices and qualified practices. In theory sessions the teacher presents the fundamentals of spectroscopic techniques, spectra and applications. The student will be evaluated continuously through the resolution of applications. In the class practice sessions the student develops, with the teacher's support, the interpretation of the spectra that belong to a certain molecule, to determine its structure. In the qualified practices the student will face alone this challenge, dominating each time the interpretation of a greater number of techniques and facing more complex challenges. In all the sessions, the active participation of the student is promoted.

VII. EVALUATION FORMULA

Calculation of the final grade (FG):

$$FG = \frac{1 * PE + 1 * FE + 1 * PA}{3}$$

PE: Partial Exam (Weight 1)
FE: Final Exam. (Weight 1)
PA: Practices Average (Weight 1)

VIII. BIBLIOGRAPHY

- Silverstein, R., F. Webster and D. Kiemle, Spectrometric Identification of Organic Compounds, 7º Ed. John Wiley & Sons, Inc., 2005, 502 págs. (Libro de Texto). Cod Bib. FC: 543.085 / S587 / 1991 (ver edición 2005).

- Sternhell, S. and J. Kalman, Organic Structures from Spectra, John Wiley & Sons, Inc., 1988, 202 págs. Cod Bib. FC: 547.346/S839.