UNIVERSIDAD DE LA RIOJA

STRUCTURAL DETERMINATION
2016-2017

Bachelor Degree:	CHEMISTRY		702G
Course title:	STRUCTURAL DETERMINATION		542
Year/Semester:	3rd/2nd	ECTS Credits:	6

DEPARTMENT

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CONTENTS

PART A. STRUCTURAL DETERMINATION OF ORGANIC COMPOUNDS.

UNIT1. Ultraviolet–visible (UV-Vis), infrared (IR) and RAMAN spectroscopies. Mass spectrometry (MS).

UNIT2. General aspects of nuclear magnetic resonance spectroscopy (NMR). Introduction and parameters

UNIT3. Proton nuclear magnetic resonance spectroscopy. Chemical shift, coupling constants and nuclear Overhauser effect.

UNIT4. Carbon-13 nuclear magnetic resonance spectroscopy and two dimensional experiments (*COSY: COrrelated SpectroscopY, TOCSY: TOtal Correlated SpectroscopY, NOESY: NOE SpectroscopY, HETCOR: HETeronuclear CORrelated spectroscopy, HSQC: Heteronuclear Simple Quantum Coherence, HMQC: Heteronuclear Multiple Quantum Coherence HMBC: Heteronuclear Multiple Bond Coherence*).

UNIT5. Structural determination of organic compounds. Resolution of problems and prediction of spectra.

PART B. STRUCTURAL DETERMINATION OF INORGANIC AND ORGANOMETALLIC COMPOUNDS.

UNIT6. Multinuclear magnetic resonance. Physical properties of nuclei.

UNIT7. Multinuclear magnetic resonance. Parameters of active nuclei in nuclear magnetic resonance.

UNIT8. Analysis and interpretation of NMR spectra.

UNIT9. Dynamic processes and nuclear magnetic resonance.

REFERENCES

Title
NMR spectroscopy in inorganic chemistry
Structural methods in inorganic chemistry
NMR, NQR, EPR and Mossbaüer spectroscopy in inorganic chemistry
Organic structures from spectra
Nuclear magnetic resonance
Spectrometric identification of organic compounds

EVALUATION SYSTEM

Tasks before final exam referred to determination of structures from spectra and simulation of spectra (20%, unrecoverable)
Final exam (70%, recoverable)
Observation techniques (10%, unrecoverable)