MASTER's DEGREE IN ADVANCED CHEMISTRY

Course Guide

Contents of the Course Guide

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COURSES:

	MASTER's DEGREE IN ADVANCED CHEMISTRY **POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY** **DEPARTMENT OF CHEMISTRY.** **FACULTY OF SCIENCES** **UNIVERSITY OF BURGOS**

COURSE			**CODE**
BOND ACTIVATION BY TRANSITION METAL COMPLEXES			5255
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (4/1)

LECTURER/S IN CHARGE OF THE COURSE			
Gabriel García Herbosa			
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LECTURER (1)			
José Vicente Cuevas Vicario			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Inorganic
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STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	20	20
	Attendance at practical classes (laboratory or computer room)	1	10
	Attendance at seminars and activities	0.6	6
	Attendance at assisted tutorials	0.5	5
	Presentation of assignments	0.5	5
	Completion of assessment tests	0.4	4
PRIVATE STUDY	Group work for theoretical and/or practical classes.	2	20
	Study for the preparation of theoretical and/or practical classes.	0.5	5
	Resolution of exercises and practical cases, preparation of reports and presentations	2.5	25
	Exam preparation.	2.5	25

Total hours (Taught Classes)	50	**Total hours (Private Study)**	75
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

Activation of N-H and O-H bonds promoted by metallic elements and directed at the catalysis of important chemical reactions.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

Students should possess knowledge of Inorganic and Organic Chemistry, satisfy the admissions criteria of the Study Plan for the Master's in Advanced Chemistry and have previously been admitted onto the course.

OBJECTIVES

General

To learn how to transmit up-to-date knowledge on the activation of O-H and N-H bonds by transition metals; to study this activation process in important catalysed reactions such as the "water gas shift", the Wacker process, "hydration" of olefins and nitrils, Hydrogen transfer to alkynes and the hydroamination of olefins.

Specific

To understand the enormous importance of water oxidative addition reactions for activation in solar energy conversion and storage schemes.
To describe the oxidative addition of amines on metals as an important step in amination processes.
To distinguish between possible mechanisms in the hydroamination process.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

The course will enable students to comprehend:

- The principal mechanisms that lead to the activation of O-H bonds.
- The principal mechanisms that lead to the activation of N-H bonds.

- Mechanisms for the formation of C-N bonds activated by transition metal complexes.
- Mechanisms for the activation of water molecules by transition metal complexes.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Oral and written communication skills in the student's 1st language.
- Oral and written communication skills in a 2nd language.
- Ability to search for and obtain information, whether through primary or secondary sources, including information obtained via on-line communication and by accessing data banks.
- Ability to summarise, and to prepare and to present reports.
- Problem-solving skills relating to qualitative and quantitative information.
- Ability to apply theoretical knowledge to professional practice.
- Abilities and skills in practical aspects, manual abilities at undertaking tasks.
- Study skills and autonomous learning, necessary for ongoing training and professional development
- Skills related to computer tools and information technology (such as word processors, spreadsheets, databases, internet communications, etc.)
- Interpersonal skills, appropriate for interpersonal relations and for integration in work groups.
- Capacity for group work.
- Decision-making capacity
- Deductive reasoning skills and the ability to exploit creative thinking, through their introduction into research.

STUDY PLAN

1. Water-based reactions with transition metal complexes in relation to their position in the Periodic Table. "Early-transition metals" and lanthanoids: Hydrolysis and reduction to hydrogen. "Late-transition metals".
2. The reaction of water oxidative additions to a metallic centre. Thermodynamic and kinetic aspects.
3. Hydride formation by reaction of metallic complexes with water.
4. Hydroamination processes catalysed by complexes of the Early-transition metals.
5. Regiochemistry in hydroamination processes.
6. The study of examples taken from the bibliography.

METHODOLOGY

Lectures coupled with the analysis and study of recent articles and assignments undertaken by students. The module is made up 40 hours of theoretical class and 10 hours of practicals. As it covers subject matter that has been developed very recently, standard reference books are not available on the coursework. Given that oxidative addition reactions and their implications for catalysis are well known, a knowledge base will be constructed on this concept in order to apply it at a later stage to cases of N-H and O-H bonding. To do so, the first stage of the teaching method will be based on well-known case studies found in works such as num. 12 (see Bibliography). The following stage will involve discussion of the articles indicated in the recommended bibliography and up-to-

date searches, also part of the teaching methods.

BIBLIOGRAPHY

Basic reference works

1. Antonio Togni, Hansjörg Grützmacher (Editors) *Catalytic Heterofunctionalization, John Wiley and Sons, ISBN:* 3-527-30234-4, 2001
2. W. N. M. Van Leeuwen *Homogeneous Catalysis*, Kluwer Academia Publishers, ISBN: 1-4020-1999-8, 2004

Other bibliographic works to consult

1. Blum, O.; Milstein, D. Journal of the American Chemical Society 2002, 124, 11456-11467.
2. Dorta, R.; Rozenberg, H.; Shimon, L. J. W.; Milstein, D. Journal of the American Chemical Society 2002, 124, 188-189.
3. Morales-Morales, D.; Lee, D. W.; Wang, Z. H.; Jensen, C. M. Organometallics 2001, 20, 1144-1147.
4. Hartwig, J. F. Pure Appl. Chem. 2004, 76, 507-516.
5. Hong, S.; Marks, T. J. Accounts Chem. Res. 2004, 37, 673-686.
6. Muller, T. E.; Beller, M. Chem. Rev. 1998, 98, 675-703.
7. Nobis, M.; Driessen-Holscher, B. Angew. Chem.-Int. Edit. 2001, 40, 3983-+.
8. Pohlki, F.; Doye, S. Chem. Soc. Rev. 2003, 32, 104-114.
9. Pryadun, R.; Sukumaran, D.; Bogadi, R.; Atwood, J. D. J. Am. Chem. Soc. 2004, 126, 12414-12420.
10. Roesky, P. W.; Muller, T. E. Angew. Chem.-Int. Edit. 2003, 42, 2708-2710.

INTERNET RESOURCES

On-line scientific journals (UBU resources). Databases (e.g. Web of Science, Current Contents, etc.)

EVALUATION

Methodology

The principal method of evaluation will be continuous assessment of the student's work, taking such aspects into consideration as active participation, questions and responses, preparation and presentation of assignments. Additionally, a written test will be set on the subject matter studied.

Marking criteria

Continuous assessment of the student's work (70%). This latter percentage comprises active participation (20%), questions and responses (10%), preparation and presentation of assignments (40 %). Additionally, a written test will be set on the subject matter studied, representing 30% of the final mark.

PROGRAMMED ACTIVITIES (Course contents and time frame)

Contents	Lecturer	Hours	
		Taught classes	Private study
1. Water-based reactions with transition metal complexes	Gabriel García Herbosa	**6**	**8**
2. The reaction of water oxidative additions to a metallic centre. Thermodynamic and kinetic aspects.	Gabriel García Herbosa	**6**	**8**

3. Hydride formation by reaction of metallic complexes with water.	Gabriel García Herbosa	**6**	**9**
4. Catalysed hydroamination processes	José Vicente Cuevas Vicario	**6**	**9**
5. Regiochemistry in hydroamination processes.	José Vicente Cuevas Vicario	**6**	**8**
6. Study of examples taken from the bibliography 1	José Vicente Cuevas Vicario	**8**	**4**
7. Study of examples taken from the bibliography 2	Gabriel García Herbosa	**8**	**4**
8. Exam preparation.		**--**	**25**
9. Completion of evaluation tests		**4**	**--**
Total	**125**		

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
INDUSTRIAL APPLICATION OF NEW MATERIALS			5243
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (4 / 1)

LECTURER/S IN CHARGE OF THE COURSE			
José Luis de la Peña Albillos			
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LECTURER (3)			
Gabriel García Herbosa			
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STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	2	30
	Attendance at practical classes (laboratory or computer room)	0.75	10
	Attendance at seminars and activities	5 h/15 wks	5
	Attendance at assisted tutorials	5 h/15 wks	5
	Presentation of assignments	5 h/15	5
	Completion of assessment tests	5/15	5
PRIVATE STUDY	Group work for theoretical and/or practical classes.	1	15
	Study for the preparation of theoretical and/or practical classes.	20/15	20
	Resolution of exercises and practical cases, preparation of reports and presentations	15	15
	Exam preparation.	15	15
Total hours (Taught Classes)	**60**	**Total hours (Private Study)**	**65**
Total hours (Taught Classes and Private Study)		**125**	

COURSE CONTENTS (DESCRIPTORS)

Polymer materials: Industrial applications. Plastics and rubber. Recycling of plastics. Metallic coatings. Polymer coatings. Energy storage. Fuel cells.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

Knowledge and understanding of fundamental aspects of mathematics, physics, and chemistry studies at graduate level.

OBJECTIVES

General

- To impart knowledge to the student on:

- The wide application range of new polymer materials.
- The incidence of polymer materials on the quality of life.
- The usefulness and possibilities of metals as coating materials.
- Modern chemical energy storage systems.

- Specific

- Aspects relating to the manufacturing industry and the processing of polymer materials.
- Plastic and rubber applications in different sectors of industrial activity – automobiles, packaging, construction, agriculture, etc-, and the recycling of those same materials.
- Devices for energy storage, based on chemical principles: materials for hydrogen storage, fuel cells, batteries,..

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

- The course will enable students to:

- Select certain materials - polymeric or metallic – in response to market and client demands.

- Select a type of processing or a treatment for a specific polymeric material in accordance with the use to which it will be put.
- Evaluate the problem of waste management and to select the most appropriate method of recycling or assessing the residues produced during industrial production or after usage.
- Select, in accordance with all possible outcomes, the most appropriate alternative for chemical energy storage systems.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Study skills and autonomous learning, necessary for ongoing training and professional development
- Skills related to numerical calculation and the use of computer tools and information and communications technology (use of word processors, spreadsheets, databases, databases internet communications, etc.)
- Ability to search for and obtain information for the preparation and presentation of reports.
- Ability to apply theoretical knowledge to professional practice.
- Ability to resolve problems that might arise in the course of daily professional activity and to put forward initiatives relating to research.
- Group work and decision-making skills

STUDY PLAN

Unit 1: New polymeric materials used in industry

Polymeric materials: Introduction.
Plastics and rubbers used in industry.
Plastics in the automotive, aeronautic and electronic industries.
Plastics in the packaging and coating sectors.
Plastics in construction and in agriculture.
Management of plastic residues: Recycling of plastics
Recycling systems: mechanical recycling, chemical recycling and energetic assessment.
Recycling by applications in industrial sectors.
Biodegradable plastic materials.
Legislation.

Unit 2: Metallic coatings

Professionals working in the industry (Group Cropu) participate by providing specialist input on metallic coatings.
Factory visit.

Unit 3: Materials and devices for energy storage

Systems for hydrogen storage.
Metallic hydrides (storage-detachment of hydrogen atoms caused by a shift in the chemical balance due to a change in pressure and/or temperature)
Saline hydrides (liberation of hydrogen by reaction with water)
Other materials for hydrogen storage (nanotubes, zeolites,…)
Fuel cells.
Batteries

Laboratory practicals:
Activities
Visit to the "Varta" battery factory

METHODOLOGY

- Lectures
- Seminars
- Presentation of assignments
- Laboratory practicals
- Tutorials
- Other activities: factory and laboratory visits, etc.

BIBLIOGRAPHY

Basic reference works

- Ciencia y Tecnología de Materiales poliméricos, Editado por Instituto de Ciencia y Tecnología de Polímeros (CSIC), Madrid, 2004
- Introducción a la química de los polímeros, R. B. Seymour, Charles E. Carraher. Reverté, Barcelona, 1995.
- Principles of polymerization, G. Odian. 3rd Ed., Wiley, New York, 1991
- Polymer synthesis and characterization: A laboratory manual, S. R. Sandler. Academic Press, San Diego 1998
- Hydrogen storage materials Barnes, R. G.; Trans Tech Publications: Aedermannsdorf, 1988.
- Synthesis and characterisation of potential hydrogen storage materials, Johansson, E.; Acta Universitatis Upsaliensis: Univ.-bibl. distributör: Uppsala, 2004

Other bibliographic works for consultation

- "Plastic Materials", J. A. Brydson. 6th Edition, Butterworth-Heinemann, London, 1995
- Industry Polymer Handbook. Products, processes, applications", vol 2, E.S. Wiiks ed., Wiley-VCH, 2001.
- "Encyclopedia of Polymer Science and Engineering", H.F. Mark, N.M. Bikales, C.G. Overberger, G., Menges, John Wiley and Sons, USA 1988.
- "Polymeric Materials Encyclopedia", vol 11, J.C. Salamon ed., CRC Press, USA 1996.
- "Comprehensive Polymer Science", vol 7, G. Alien, J.C. Bovington, eds., Pergamon, Oxford 1989
- "Additives for Plastics Handbook", J. Murphy ed., Elsevier Advance Technology, Oxford UK 1996
- "Paints and Surface Coatings. Theory and Practice" 2nd ed., R. Lambourne, T.A. Stevens eds., William Andrew Publishing, USA 1999

INTERNET RESOURCES

http://www.ubu.es/biblioteca/resources_inet/estadistica_m.htm
http://www.polymersdatabase.com/

ASSESSMENT

Methodology

- Preparation and presentation of reports
- Preparation of assignments
- Resolution of exercises and practical cases
- Participation in seminars, tutorials and other activities
- Completion of assessment tests
- Final Exam

Marking criteria

-	Preparation and presentation of reports	40%
-	Resolution of exercises and practical cases	15 %
-	Participation in seminars, tutorials and other activities	15 %
-	Completion of written tests	30 %

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1.- New polymeric materials used in industry	José Luis de la Peña /José Miguel García	20	17
Unit 2.- Metallic coatings	Gabriel García Herbosa	10	9
Unit 3.- Materials and devices for energy storage	Gabriel García Herbosa /José Miguel García	13	11
Activities and practicals:	José Luis de la Peña /José Miguel García	12	11
Exam preparation.		--	17
Completion of assessment tests		5	--
Total	**125**		

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POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY.
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS.

COURSE			CODE
ADVANCES IN NEW MATERIALS (I)			5244
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	2	Semi-optional	5 (4/1)

LECTURER/S IN CHARGE OF THE COURSE			
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Nicolás Alejandro Cordero Tejedor			
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Begoña Torres Cabrera			
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LECTURER (5)			
Tomás Torroba Pérez			
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STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	35/15	35
	Attendance at practical classes (laboratory or computer room)	10/15	10
	Attendance at seminars and activities	5/15	5
	Attendance at assisted tutorials	5/15	5
	Presentation of assignments	1	15
	Completion of assessment tests	5/15	5
PRIVATE STUDY	Group work for theoretical and/or practical classes.	1	15
	Study for the preparation of theoretical and/or practical classes.	1	15
	Resolution of exercises and practical cases, preparation of reports and presentations	1	15
	Exam preparation.	5/15	5
Total hours (Taught Classes)	75	**Total hours (Private Study)**	50
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

Special polymers: Electrosynthesis and characterisation of polymer conductors. Polymer applications in the field of sensors. Synthesis and properties of organic molecular materials. Nanometric structures. Metallic aggregates.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

In order to follow the subject matter on the course satisfactorily it is recommended that the student possess a basic understanding of polymer synthesis and its properties and applications, as well as knowledge of the fundamental principles of organic and inorganic synthesis, electrochemistry and the main instrumentation techniques in chemistry.

OBJECTIVES

General

- To offer the student a view of a basic and an applied nature of certain advances in the science of materials and their applications in various technological fields, such

as sensors, nanotechnologies, polymer conductors and metallic aggregates.
- To introduce the student to the challenges of the 21st C. in the field of New Materials related to the control, handling and design of nanometric-sized materials, intelligent materials and biomimetic materials.
- To provide the student with a global view of some cutting-edge fields of the Science of materials with considerable industrial impact.

- Specific

- To enable the acquisition of knowledge on the relation between the processes of obtaining materials of technological interest, their microstructure and their final properties.
- To understand the fundamentals of the phenomena that govern the behaviour of the different materials under study and the variables that define it.
- To know how to apply the concepts under study to the resolution of problems relating to the determination of variables that affect a material's behaviour and their application in the selection of relevant materials.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

- The course will enable students to:

- Understand the relation between macroscopic properties and the properties of individual atoms and molecules: including macromolecules, colloids and other materials.
- Resolve qualitative and quantitative problems according to a previously developed model.
- Recognise and analyse new problems and establish strategies to solve them.
- Plan, design and execute practical research, from the problem-recognition stage up until the evaluation and assessment of the results and discoveries.
- Recognize and assess chemical processes in daily life.
- Interrelate different disciplines (chemistry, physics, engineering).
- Develop a critical and self-critical capacity.
- Generate new ideas.

– GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Analytical and summary skills
- Organisational and planning skills
- Oral and written communication skills in the student's 1st language.
- Information management skills
- Problem-solving skills
- Ability to work in an interdisciplinary group
- Interpersonal relationship skills
- Ethical compromise
- Autonomous learning skills
- Ability to adapt to new situations
- Creativity
- Initiative and a spirit of enterprise
- Quality-driven approach
- Sensitivity towards environmental issues

STUDY PLAN

Unit 1 Polymer material sensors.
- Polymers with special applications.

- Molecular sensors.
- Conventional materials used in the field of sensors.
- Polymer materials in gas detection systems, temperature sensors, humidity sensors, ion-selective sensors, pH sensors, systems to detect organic substances, biosensors.

Unit 2 Electrosynthesis and characterisation of conducting polymers.

- General aspects of conducting polymers. Some representative examples. P-doping and n-doping. Conductivity and electrochromaticity.
- Electrochemical synthesis of conducting polymers.
- Analytical tools in electrosynthesis and characterization of electrogenerated polymers.
- Electron transfer mechanisms in polymer-dissolution systems.

Unit 3 Carbon Nanostructures.

- Introduction: Carbon materials.
- The synthesis of carbon nanostructures.
- Fullerenes (geometry, electronic structure, properties).
- Nanotubes (geometry, electronic structure, properties).
- Other structures (nanocords, nano-onions, nanohorns...).

Unit 4 Metallic aggregates.

- Stability and magical numbers of aggregates.
- Alcaline metallic aggregates. Electronic structure and the Jellium model.
- The importance of geometry and the Spherically Averaged Pseudopotential (SAPS) model.
- Aggregates of noble metals: geometries and properties.

Unit 5 Organic molecular materials.

- New Organic Materials.
- Organic material conductors of electricity: Polymer conductors, Organic molecular metal macrocycles and electroactive molecules.
- Organic superconductors
- Liquid crystals
- Dendritic molecules

METHODOLOGY

a) Taught classes

The active participation of students is indispensable in the orderly presentation of concepts for them to integrate into one single scheme not only their prior knowledge (appropriately corrected and completed), but also the key ideas of the thematic block and the concepts drawn from other subjects that the student might be studying at the same time.

The variety and relative complexity of some of the concepts requires the use of teaching devices such as projectors for graphs and equations (transparencies, animations) as well as the study of selected bibliographic items, which are provided to the student as classroom discussion material.

b) Individual or group work.

This is based on the search for available bibliographic sources of information and on the preparation of reports, not necessarily original, on complementary topics.

BIBLIOGRAPHY

Basic reference works
- G. Harsanyi, "Polymer Film in Sensor Applications", Gabor, CRC Press, 1995. - G. G. Wallace, G.M. Spinks, L.A.P. Kane-Maguire and P.R. Teasdale, "Conductive Electroactive Polymers. Intelligent materials systems." CRC Press (2nd ed.), 2003. - A.F. Díaz, M.T. Nguyen and M. Leclerc, "Electronicallly Conducting Soluble Polymers" en Physical Electrochemistry, I. Rubistein Ed., Marcel Dekker, 1995. - M.S. Dresselhaus, G. Dresselhaus and P.C. Eklund, "Science of fullerenes and carbon nanotubes", Academic Press, 1996. - W. A. De Heer, Reviews of Modern Physics 65, 611 (1993). - M. Brack, Reviews of Modern Physics 65, 677 (1993). - J. P. Farges ed. "Organic Conductors. Fundamentals and Applications", Marcel Dekker, New Cork, 1994. - F. Vögtle, "Supramolecular Chemistry", Wiley, 1991. - P. J. Collings and M. Hird, "Introduction to Liquid Crystals", Taylor & Francis, London, 1997. - J. Williams et al., "Organic Superconductors (Including Fullerenes)", Prentice Hall, N.J., 1992.
Other bibliographic works to consult
- Y. Osada, D.E. De Rossi, "Polymer Sensor and Actuators", Springer, 2000. - B. Adhikari, S. Majumdar, Polymer in Sensor Applications, Prog. Polym. Sci, 29, (2004), 699-766. - J.F. Rubinson and H.B. Mark (Eds.), "Conducting Polymers and Polymer Electrolytes. From Biology to Photovoltaics", ACS Synposium Series 832, ACS, 2003. - J. Roncali, Chem. Rev. 92 (1992), 711-738 - Carbon Nanotubes: Synthesis, Structure, Properties and Application, M.S. Dresselhaus, G. Dresselhaus and P. Avouris (eds), Springer Verlag, 2000. - R. Saito, G. Dresselhaus and M.S. Dresselhaus, "Physical properties of carbon nanotubes", Imperial College Press, 1998. - P.W. Fowler and D.E. Manolopoulos, "An atlas of fullerenes", Oxford University Press, 1995. - Metal Clusters, W. Ekardt (Editor), Wiley Series in Theoretical Chemistry. - W.A. de Heer, W.D. Knight, M. Y. Chou, M. L. Cohen, Solid State Physics 40, 93. - N. Martín, C. Seoane, "From Electrón Aceptor Molecules to Photoinduced Intramolecular Charge Transfer Complexes", Ch. 1, in Handbook of Electrically Conducting Molecular and Polymeric Materials. N. S. Nalwa, ed. Wiley, 1997. - C. C. Leznoff, A. B. P. Lever, "Phthalocyanines. Properties and Applications", VCH. "Burgos- New York" 1989-1993. 1-4.

INTERNET RESOURCES
• http://acronyms.thefreedictionary.com/Conducting+polymer • http://en.wikipedia.org/wiki/Conductive_polymers • http://nobelprize.org/chemistry/educational/conductive_polymers/

- http://www.pa.msu.edu/cmp/csc/nanotube.html
- http://www.geocities.com/upwardthrust/carbon/fullerene.html
- http://fysik5.fysik.uu.se/research/clusters/clusters.html

ASSESSMENT
Methodology
- Theoretical and practical tasks (individual or group work). - Participation in seminars, tutorials and other activities - Completion of assessment tests
Marking criteria
The attainment of objectives will be evaluated in accordance with the following criteria: - Theoretical and practical tasks (individual or group work). (40%) - Participation in seminars, tutorials and other activities (30%) - Completion of assessment tests (30%)

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1	Félix C. García García	14	9
Unit 2	Jesús López Palacios	14	9
Unit 3	Nicolás A. Cordero Tejedor	14	9
Unit 4	Begoña Torres Cabrera	14	9
Unit 5	Tomás Torroba Pérez	14	9
Exam preparation.		--	5
Completion of final assessment test		5	--
Total		**125**	

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
ADVANCES IN NEW MATERIALS (II).			5245
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	2	Semi-optional	5 (4/1)

LECTURER (1) IN CHARGE OF THE COURSE			
Javier García Tojal			
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LECTURER (3)			
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LECTURER (4)			
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STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	2.5	38
	Attendance at practical classes (laboratory or computer room)	1.6	24
	Attendance at seminars and activities	0.2	3
	Attendance at assisted tutorials	0.1	2
	Presentation of assignments	0.3	4
	Completion of assessment tests	0.3	4
PRIVATE STUDY	Group work for theoretical and/or practical classes.	0.3	5
	Study for the preparation of theoretical and/or practical lessons.	0.7	10
	Resolution of exercises and practical cases, preparation of reports and presentations	1.7	25
	Exam preparation.	0.7	10
Total hours (Taught classes)	75	**Total hours (Private Study)**	50
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

- Thermal analysis of new materials.
- Principles of fluorescence.
- Materials and fluorescent probes.
- Optical materials, semiconductors and superconductors.
- New magnetic materials.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

It is recommended that the student possess knowledge of physics and chemistry at graduate level.

OBJECTIVES

General

- To understand the basic principles of the properties under study.
- To understand which materials present specific properties and their most important applications.
- To become familiar with different types of techniques that serve to characterize the properties of a material while remaining aware of their limitations
- To apply methods and experimental techniques under study in order to characterize the properties and applications of new materials.
- To keep up with cutting-edge research in the field of new materials.

Specific

- To design compounds that present particular optical, electrical, thermal or magnetic properties.

- To characterize the thermal, luminescent, optical, electronic and magnetic behaviours of a material.
- To establish a structure-properties correlation for each type of material.
- To identify the characteristics of a material that make it appropriate for industrial applications.

To discuss the results obtained from the characterization of a new material and develop an ability to design new systems and/or experiments which will give further information on the material under study.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

The course is intended to enable students to:

- Gain sufficient knowledge to approach the study of a new material that presents particular optical, electrical, thermal, or magnetic properties.
- Learn how to acquire, analyse and interpret thermal, electrical, optical, photophysical and magnetic data.
- Become aware of the possibilities and limitations of a new material, as well as the most appropriate techniques for its characterization.
- Understand the applications of new materials in relevant fields, and principally in the industrial field.
- Acquire abilities and systematic approaches to the synthesis and characterization of a new material in the laboratory.
- Develop laboratory work in accordance with safety regulations and respect for the environment.
- Critically apply scientific methods to the theoretical and experimental study of new materials.
- Write technical reports that may be easily understood by anyone with a scientific background.
- Make a presentation and lead a group discussion on the results of a study on the thermal, electrical, optical, photophysical or magnetic properties of a material.
- Gain sound theoretical and experimental experience in characterizing and preparing new materials to give the students the basic skills to develop further in this field.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Oral and written communication skills in the student's mother tongue.
- Use of bibliographic sources and databases.
- Ability to analyse data, to sum up results, and to prepare and present reports.
- Problem-solving skills applied to qualitative and quantitative information.
- Ability to apply the acquired theoretical knowledge.
- Abilities and skills in all practical aspects related to laboratory work.
- Study skills and autonomous learning skills necessary for ongoing training and professional development
- Computing skills related to computer tools and information technology.
- Interpersonal skills, appropriate for cultivating positive interpersonal relationships and for integration in work groups.
- Decision-making capacity
- Ability to integrate quality as one of the most important variables to be considered.
- Deductive reasoning skills and the ability to apply creative thinking to scientific research.

- Ability to recognise aspects related to occupational safety and environmental impact as fundamental aspects of their professional conduct.

STUDY PLAN

Unit. 1. Thermal analysis of new materials.
General concepts and application to new materials: DSC (Differential Scanning Calorimetry), TGA (Thermogravimetric Analysis), TMA (Thermo Mechanical Analysis), DMA (Dynamic Mechanical Analysis).

Unit 2. Materials and fluorescent probes.
Study of the interaction between radiation and matter. Photophysical processes. Fluorescence. Equipment. Effects on the environment. Quenching and energy transference processes. Flurorescent probes and their applications. Emitting polymers.

Unit 3. Optical materials, semiconductors and superconductors.
Non-linear optics. Piezooptical, electrooptical and magneto-optical materials. Semiconductors. Thermal and optoelectric effects. Superlattices. Applications. Superconductivity. Josephson junctions. High temperature superconductors.

Unit. 4. New magnetic materials.
Factors that determine the magnetic behaviour of a compound. Types of magnetic materials and applications. Design and synthesis of organic and inorganic magnetic materials.

Unit 5. The interdisciplinary laboratory.
Preparation of heterodinuclear complexes that simultaneously incorporate d and f-block metallic ions. Follow up of the synthesis reaction by electronic spectrography (absorption and emision). Luminiscent, optical, magnetic and thermal properties.

METHODOLOGY

- Lectures at which the foundation, objectives and working methods are set out for each of the course contents.
- Development of the work in three stages: (i) fundamental aspects of the properties under study; (ii) case by case study; (iii) application to practical problems and examples.
- Organisation of participative seminars in which students become familiar with the theoretical content of the course.
- Interdisciplinary laboratory work in different scientific areas.
- Preparation and presentation of reports
- Individual selection of a topic and preparation of an assignment on the same subject guided by the subject lecturers.

BIBLIOGRAPHY

Basic reference works

1. J. S. Miller, M. Drillon (Ed.), "*Magnetism: Molecules to Materials*", Wiley-VCH, Weinheim, 2001-2004. (Vols. I–V).
2. K. Itoh, M. Kinoshita, "*Molecular Magnetism: New Magnetic Materials*", Kodansha and Gordon & Breach, Tokyo-Amsterdam, 2000.
3. O. Kahn, "*Molecular magnetism*", VCH Publishers, Weinheim, 1993.
4. J. R. Lakowicz, "*Principles of Fluorescence Spectroscopy*", 2ª Ed., Plenum Publsihers, Nueva York, 1999.
5. N. J. Turro, "Modern Molecular Photochemistry", University Science Books, California, 1991.

6. W. Rettig, B. Strehmel, S. Schrader, H. Seifert (Eds.) "Applied Fluorescence in Chemistry, Biology and Medicine", Springer, New York, 1999.
7. P. J. Haines (Ed.), "*Principles of Thermal Analysis and Calorimetry*", The Royal Society of Chemistry, London, 2002.
8. R.W. Boyd, "*Nonlinear Optics*", Academic Press, 1992.
9. C. Kittel, "*Introduction to Solid State Physics*", Wiley and Sons, New York, 1996.

Other bibliographic works to consult

1. P. Day, A. E. Underhill (Ed.), "*Metal-Organic and Organic Molecular Magnets*", Royal Society of Chemstry, London, 2000.
2. W. Linert, M. Verdaguer (Ed.) "*Molecular magnets: recent highlights*", Springer-Verlag, Vienna, 2003.
3. J. R. Rabek, "*Photochemistry and Photophysics*", Volumen I y II, CRC Press, Florida, 1990.
4. K. K. Rohatgi-Mukherjee, "*Fundamentals of Photochemistry*", Wiley Eastern Limited, Nueva Deli, 1988.
5. "*Encyclopedia of Materials: Science and Tecnology*", SCIENCE@direct, 2005.
6. Costes, J.-P.; Dahan, F.; Dupuis, A.; Laurent, J.-P. *Chem. Eur. J.* 1998, *4*, 1616-1620.
7. Costes, J.-P.; Dahan, F.; Dupuis, A. *Inorg. Chem.* 2000, *39*, 165-168.
8. Costes, J.-P.; Dahan, F.; Dupuis, A.; Laurent, J.-P. *Inorg. Chem.* 2000, *39*, 169-173.
9. G. Strobl, "*Condensed Matter Physics: crystals, liquids, liquid crystals and polymers*", Springer, New York, 2003.
10. R. Guenther, "*Modern Optics*", Wiley and Sons, New York, 1990.
11. L. Mandel and E. Wolf, "*Optical Coherence and Quantum Optics*", Cambridge University Press, Cambridge, 1995.

INTERNET RESOURCES

- http://www.fluorescence-resource.com/
- http://en.wikipedia.org/wiki/Fluorescence/
- http://micro.magnet.fsu.edu/primer/techniques/fluorescence/fluorescenceintro.html
- http://scienceworld.wolfram.com/physics/Fluorescence.html
- http://johnbokma.com/pet/scorpion/detection-using-uv-leds.html/
- http://superconductors.org/
- http://www.csr.umd.edu/
- http://phys.strath.ac.uk/12-370/
- http://home3.netcarrier.com/~chan/MATERIAL/
- http://www.mse.cornell.edu/courses/engri111/magnet.htm
- http://www.aacg.bham.ac.uk/magnetic_materials/type.htm
- http://www.school-for-champions.com/science/magnetic_materials.htm

ASSESSMENT

Methodology

- Continuous assessment of training and learning outcomes evaluating each student's progress on the basis of:
  a) The resolution of exercises and practical cases.
  b) Participation in seminars, tutorials and other activities.
  c) Performing laboratory work.
  d) Preparation and presentation of reports.
  e) Preparation, presentation and defence of an individual assignment.
- Final assessment: A final written test on all the subject matter will be set.

Marking criteria

– Continuous evaluation. 40%

This mark represents an evaluation of the active participation of the student, the answers given in the theoretical-practical cases, the development of laboratory work and, where applicable, the preparation and presentation of reports.

- Final exam 30%
  A four-hour final written exam on all of the subject matter, involving the resolution of questions and selected problems.
- Preparation, presentation and defence of an individual report. 30%
  Each student will prepare a written assignment, which must be presented in public (for 30 minutes) and defended in front of the course lecturers. The subject must be chosen from among those put forward by the lecturers.

PROGRAMMED ACTIVITIES (Course contents and time frame)

Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit. 1.-. Thermal analysis of new materials.	Begoña García	14	8
Unit 2.-. Materials and fluorescent probes.	María José Tapia	14	8
Unit 3.-. Optical materials, semiconductors and superconductors.	Ángel Ballesteros	14	8
Unit. 4.-. New magnetic materials.	Javier García	14	8
Unit 5.-. The interdisciplinary laboratory.	All lecturers	15	8
Exam preparation.		--	10
Completion of final assessment test		4	--
Total		**125**	

	MASTER's DEGREE IN ADVANCED CHEMISTRY **POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY** **DEPARTMENT OF CHEMISTRY** **FACULTY OF SCIENCES** **UNIVERSITY OF BURGOS**

COURSE			**CODE**
QUALITY CONTROL AND ASSURANCE IN PROCEDURES, PROCESSES AND PRODUCTS.			5249
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (3T/2P)

LECTURER (1) IN CHARGE OF THE COURSE			
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LECTURER (2)			
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STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	1	15
	Attendance at practical classes (laboratory or computer room)	5	30
	Attendance at seminars and activities	5/15	5
	Attendance at assisted tutorials	5/15	5
	Presentation of assignments	2/15	2
	Completion of assessment tests	3/15	3
PRIVATE STUDY	Group work for theoretical and/or practical classes.	1	15
	Study for the preparation of theoretical and/or practical classes.	25/15	25
	Resolution of exercises and practical cases, preparation of reports and presentations	1	15
	Exam preparation.		10
Total hours (Taught Classes)	60	**Total hours (Private Study)**	65
Total hours (Taught Classes and Private Study)	125		

CONTENTS (DESCRIPTORS) OF THE COURSE

Accreditation of testing and calibration laboratories. Validation of chemical measurements. Control of toxic and prohibited residues. Product and process controls. Process capability. Multivariate control. Process analytical Technology (PAT).

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

It is recommended that students possess: a basic knowledge of basic statistics and procedures in analytical chemistry and instrumental chemical techniques.

OBJECTIVES

General

To understand the need for an objective methodology to control a procedure, a process or a product
To understand statistical methodology to validate a measure and/or an effect
To understand the need for and the utility of robust methodology
To understand univariate and multivariate control charts, their meaning, validation and use.

Specific

To know how to provide an analytical measure of certainty.
To compare results in a range of concentrations.
To use confidence intervals and hypothesis tests in order to confirm the analytical measure.
To use ANOVA (Analysis of Variance) methods to identify significant effects in the factors whether fixed or random.
Breakdown the total variability of a process into the sum of its components.

To construct nested ANOVA.
To determine appropriate sampling sizes for preset powers of tests.
To detect outlier data through appropriate robust techniques in both inter-laboratory assays as well as by using regression techniques.
To determine the repeatability and reproducibility of a procedure.
To construct a calibration model signal as a function of concentration for all types of analytical instrumentation.
To construct univariate control charts for centralization and dispersion measurements.
To construct confidence intervals for the mean, standard deviation and range for the construction of control charts.
To estimate the covariances matrix for T^2-based multivariate charts.
To use control chart operating curves based on different probability distributions.
To use Poisson, normal and binomial distributions.
To construct control charts setting the limits for Acceptable Quality Limit (AQL), and Limiting Quality (LQ), Average Outgoing Quality Limit (AOQL) or by selecting the Operating Characteristic (OC) curve.
To calculate the OC curve of a preset acceptance sampling plan.
To study heterogeneity in batches.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

The course will enable the student to:

Become aware of international norms on chemical measurements and good laboratory practices.
Adjust measurement processes to quality objectives and continuous improvement.
Contribute solutions to problems in the same terms as they are expressed.
Evaluate, interpret, and summarise chemistry-related data and information.
Implement good scientific practice in measurement and experimentation.
Operate specific software.
Follow up qualities, events or changes in the material (reliability and robustness).
Use evaluation and auditing techniques.
Take objective decisions under uncertainty conditions.
Understand error transmission in analytical measurement.
Analyse process capacity.
Design sampling plans for attributes or for variables.
Construct and interpret control charts.
Construct confidence intervals through computer-intensive techniques (bootstrap resampling).
Establish the robustness of a procedure through "a priori" designs (Hadamard designs)
Plan, design and execute (develop) practical research from the problem recognition stage through to the evaluation of results.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Deductive reasoning skills and the application of creative thinking, through its introduction into applied research.
- Analytical skills and an ability to summarise.
- Ability to organise and to adapt to new situations.
- Report presentation and preparation skills.
- Oral and written communication skills in the student's 1st language.
- Capacity to implement different technical aspects in the field of work.

- User knowledge of computing tools and information technology.
- Abilities involving the application of theoretical knowledge in practical work.
- Aptitude for autonomous learning and self-study.
- Ability to search for and obtain information, whether from primary or secondary sources, including information obtained through on-line communication and through access to data banks.
- Integration into work groups, above all interdisciplinary ones.
- Critical reasoning and capacity for self-evaluation.
- Concern for quality.

STUDY PLAN

Unit 1. Accreditation of testing and calibration laboratories.
General accreditation criteria for testing and calibration laboratories according to ISO, EN, and UNE norms. Quality assurance policy: Quality systems, standard work protocols. Quality assessment and control: Audits, comparison of results, control samples. Accreditation concepts, certification and homologation. Types of comparative tests: Aptitude tests (intercomparison, intercalibration), collaborative studies (to adopt/compare methods), certification studies (reference material and reference certification)

Unit 2. Validation of chemical measurements.
2.1. Metrology of chemical measurements
Measurement models in chemical analysis. Systematic and random errors. Figures of merit in analytical validation: accuracy, trueness, precision, repeatability, reproducibility, analytical sensitivity, linear range, detection limit, robustness, reliability and traceability. Basic statistical tools to evaluate these figures of merit: confidence intervals, hypothesis test, ANOVA, regression. The viewpoint of certain norms and institutions: ISO, EN, UNE, AOAC, IUPAC, Harmonised Protocol, EURACHEM, etc.

2.2. Confidence intervals, Hypothesis test
Type I and II errors (α and β). Evaluation of the power of the test and calculation of the sampling sizes. Test to contrast a mean value or a variance against a reference value. Comparison of two analytical procedures for precision and trueness. T-test for paired measurements. Introduction to robust, non-parametric tests. Computer-intensive-based intervals and tests.

2.3. Variance analysis
Comparison of more than two procedures. Analysis of variance (ANOVA). Evaluation of repeatability and reproducibility according to the ISO 5725 norm. Calculation of the ANOVA power and sampling sizes. Multiple mean tests. ANOVA of more than one factor. ANOVA with nested factors. Variance components. Non-parametric alternatives.

2.4. Univariate calibration
Least-squares linear regression models. Validation of the model. Confidence intervals. Analytical sensitivity, linear range and detection limit. Detection capability according to the ISO 11843 and IUPAC norms. Risk of false positives and false negatives. Comparison of two or more calibration slopes. Comparison of analytical procedures in a given concentration range. Detection of outlier data through robust regression based on the median of squares. Other alternatives.

2.5 Control of toxic and prohibited residues.
Operational characteristics of qualitative and quantitative methods. Operational criteria with maximum residue limits (MRL) in accordance with European norms. Evaluation of CCα and CCβ. Criteria for the identification of minimum levels of prohibited substances

when chromatographic, spectroscopic and other techniques are used.

Unit 3. Product and process controls.
3.1. Process controls
Process controls by variables. Control charts for the mean, for the standard deviation and ranges. Control charts for attributes. Control charts for a binomial (number of items, "defectives", proportions, percentages). Control charts for the number of defects (λ parameter of the Poisson distribution). Process control plan designs by variables and by attributes. Operative curves. Analysis of tendencies through mobile measurement, accumulative techniques (Cusum). Robust methodology in control charts.

3.2. Process capacity
Nominal values and specifications. Estimation of the probability outside of specification. Capacity indices under the normal hypothesis. Tolerance intervals for certain distributions: normal, exponential, log-normal, Weibull. Tolerance for free and/or non-parametric distributions. Control by attributes: operative curves, multiple and sequential sampling plans. Quality indicators: Acceptable quality level (AQL), Limiting quality (LQ), Average Output Quality (AOQ). Design of a sampling plan. Standardised plans: MIL-STD-105D (ISO 2859). Continuous production: MIL-STD 1235B. Control by variables: Designs with known standard deviation: MIL-STD-414 (ISO 3951)

Unit 4. Multivariate analysis in product and process controls.
4.1. Multivariate control.
The problem of correlation between variables. Multivariate control charts based on Hotelling's T^2. Multivariate analysis in process analysis technology. Decomposition techniques based on principal components and on parallel factor (PARAFAC) analysis in the control process. Process controls based on Partial Least Squares (PLS) and similar techniques.

4.2. New tendencies in analytical control processes (Process Analytical Technology - PAT)
On-line spectroscopic techniques. Near infrared (NIR), Millimeter-wave Imaging Radiometer (MIR), Raman, Ultraviolet-Visible, and image analysis techniques. Off-line techniques: chromatography, spectroscopy, electrochemistry, etc. Applications in the production of pharmaceutical products, foodstuffs and polymers.

METHODOLOGY

The subject is developed by interposing the fundamental theoretical and practical knowledge necessary for the resolution of problems, through real data such as case studies and the use of specific professional software to reach the set objectives (Statgraphics and others). Once the fundamental theoretical aspects are understood and having confirmed that they have been correctly applied to the resolution of the proposed problem, a shared debate is held on the results and the conclusions obtained, and the path to follow, if the problem so requires. This sequence of events will allow progress to be made on the construction and assimilation of the student's own knowledge of the subject matter, and the generation and appropriate follow up in the chemical analysis laboratory of their own experimental data. The results will be evaluated through individual written reports that will be defended in front the other students.

BIBLIOGRAPHY

Basic reference works

- R. Brerenton. Data Analysis for the Laboratory and Chemical Plant. John Wiley, New

York, 2003.
- H. Martens, Magni Martens. Multivariate Analysis of Quality: An Introduction. Wiiks ed., Wiley-VCH, 1999.
- T. Naes, T. Isaksson, T. Fearn and T. Davies Multivariate Calibration and Classification, NIR publications, Chichester UK, 2002.
- D.L, Massart, B.G.M. Vandeginste, L.M.C. Buydens, S. de Jong, P.J. Smeyeers-Verbeke, Handbook of Chemometrics and Qualimetrics; Part A and Part B in Data Handling in Science and Technology, Elsevier, Amsterdam, 1997.
- N. Draper and H. Smith, Applied Regression Analysis, 3ª ed. John Wiley, New York, 1998.
- K. Bakeev, Ed. Process Analytical Technology. Blackwell Publishing, Oxford UK, 2005.
- Analytical Quality Assurance and Good Laboratory Practice in Dairy Laboratories, International Dairy Federation Special Issue num. 99302. International Dairy Federation, Brussels, 1993.
- P. James, Gestión de la Calidad Total, Prentice Hall, Madrid, 1997.
- G. Kateman, L. Buydens, Quality control in Analytical Chemistry, Wiley-Interscience, New York, 1993.

Other bibliographic works to consult

- R. Kellner, J. M. Mermet, M. Otto and H. M. Widmer. Analytical Chemistry: The approved text to the FECS curriculum analytical chemistry, Ed.Wiley-VCH, 1998.
- M. Otto. Chemometrics Statistics and Computer Applications in Analytical Chemistry, Wiley-VCH, 1999.
- ISO 17025; General requirement for the competence of calibration and testing laboratories.,1999
- ISO 3534-1 Statistical Methods for quality control. Vol 1 vocabulary and symbols.,2003
- ISO 5725, Accuracy (trueness and precision of measurements methods and results), 1994.
- ISO 11843 Capability of detection. Part.II: Methodology in the linear calibration case, 2000.
- L. Sach, Applied Statistics, Springer-Verlag, New York, 1982.
- F.W. Breyfogle, Implementing SIX SIGMA, Smarter Solution Using Statistical Methods, John Wiley, New York, 1999.
- C.Pérez Muestreo estadístico, conceptos y problemas resueltos. Pearson education S.A., Madrid, 2005.
- R.L. Scheaffer, M. Franadesikan, A. Watkins, J.A. Witmer. Activity-Based Statistics, Springer Verlag, New York, 1996.

INTERNET RESOURCES

http://www.iso.org/
http://www.iupac.org/
http://www.aenor.es
http://www.aoac.org/
http://www.eurachem.ul.pt/index.htm/
http://www.quality.org/

ASSESSMENT

Methodology

- Preparation and presentation of reports
- Preparation of assignments
- Resolution of exercises and practical cases
- Participation in seminars, tutorials and other activities

- Completion of a individual assessment test at the end of the course
Marking criteria
- Preparation and presentation of reports, 20% - Preparation of assignments, 20% - Resolution of exercises and practical cases, 20% - Participation in seminars, tutorials and other activities, 15% - Completion of a individual assessment test at the end of the course, 25%

PROGRAMMED ACTIVITIES (Subject matter and Time frame)

Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1. Accreditation of testing and calibration laboratories.	M.Cruz Ortiz Luis Sarabia Ana Herrero Mª Sagrario Sánchez	2	4
Unit 2. Validation of chemical measurements.		27	25
Unit 3. Product and process controls.		14	13
Unit 4. Multivariate analysis in product and process controls.		14	13
Exam preparation.		--	10
Completion of final assessment test		3	--
Total	125		

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
POLYMER MATERIALS: SYNTHESIS, PROPERTIES AND APPLICATIONS			5246
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (4/1)

LECTURER (1) IN CHARGE OF THE COURSE			
José Miguel García Pérez			
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LECTURER (2)			
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LECTURER (3)			
José Luis de la Peña Albillos			
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STUDENT WORKLOAD		HOURS	
		Weekly	Total
⊳ ⊣	Attendance at lectures	2	30

	Attendance at practical classes (laboratory or computer room)	10/15	10
	Attendance at seminars and activities	5/15	5
	Attendance at assisted tutorials	5/15	5
	Presentation of assignments	5/15	5
	Completion of assessment tests	5/15	5
PRIVATE STUDY	Group work for theoretical and/or practical classes.	1	15
	Study for the preparation of theoretical and/or practical classes.	20/15	20
	Resolution of exercises and practical cases, preparation of reports and presentations	15	15
	Exam preparation.	15	15

Total hours (Taught Classes)	**60**	**Total hours (Private Study)**	**65**
Total hours (Taught Classes and Private Study)		**125**	

COURSE CONTENTS (DESCRIPTORS)

The concept of the polymer. Polymer families. Polymerisation processes. Plastics. Rubber. Elastomers. Polymer properties.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

The student is expected to possess a sound knowledge and understanding of basic aspects of mathematics, physics, and chemistry at graduate level.

OBJECTIVES

General

Impart knowledge to the student on:

- The composition and behaviour of polymers.
- Families of synthetic polymers, their methods of synthesis and their properties
- The nature, properties and applications of rubbers and elastomers.

Specific

- The basic concepts of the composition and classification of synthetic polymers.
- The physical properties, mechanical behaviour, and thermal transitions of polymers.
- Methods of synthesis and polymerisation techniques, as well as procedures for the modification, degradation and stabilisation of synthetic polymers and rubbers.
- Processing methods and applications of plastics and of rubbers

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

The course will enable the student to:

- Acquire a sound knowledge of polymer structures.
- Acquire a sound knowledge of the main families of polymers, their structures and preparation methods.
- Understand the close relation existing between the chemical structure of a polymer and its properties.
- Recognise the wide range of synthetic polymer applications, according to the design of their properties, in different scientific and industrial fields.

- Treat and use polymer materials polymer appropriately.
- Propose the use of plastics and rubbers as against other materials, such as metals for example.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Study skills and autonomous learning, necessary for ongoing training and professional development
- Skills related to numerical calculation and the use of computer tools and information and communications technology (use of word processors, spreadsheets, databases, databases internet communications, etc.)
- Ability to search for and obtain information for the preparation and presentation of reports.
- Skills involving the application of theoretical knowledge in professional practice.
- Capability to resolve problems that might arise in the course of daily professional activity and to propose research-related initiatives.
- Group work and decision-making skills

STUDY PLAN

Unit 1. The composition and behaviour of polymers.

Basic concepts on the composition and classification of polymer materials.
Polymerisation and polymerisation techniques.
Polymer characteristics.
Aggregation states and thermal transitions.
Mechanical behaviour of polymer materials.
Rheology of polymer melts.
Modification, degradation and stabilisation of polymers.

Unit 2. Families of synthetic polymers: Synthesis and properties.

Polymer additives: Polyolefins, acrylic polymers, styrene polymers and polyvinyl chloride.
Condensation polymers: Polyesters, polyamides, resins and polyurethanes.
Other polymers: Hydroxylic polymers, silicones, electroactive polymers and liquid crystals.

Unit 3. Rubbers and elastomers.

Natural rubber and synthetic rubbers.
Formulation of rubber mixtures: Ingredients.
Thermoplastic elastomers: Composition and characteristics.

Unit 4. Polymeric material processing methods.

Processing of thermoplastics: Extrusion and injection.
Processing of thermostable materials: Molding techniques:
Rubber and elastomer processing methods.

Activities

- Laboratory practicals
- Seminars

- Visits to factories that produce, or use polymeric materials for different purposes.
- Visits to Centres or Laboratories conducting material analyses.

- Visits to waste purification, and sewage treatment plants.

METHODOLOGY

- Lectures
- Seminars
- Presentation of assignments
- Laboratory practicals
- Tutorials
- Other activities: Factory and laboratory visits, etc.

BIBLIOGRAPHY

Basic reference works

- Ciencia y Tecnología de Materiales poliméricos, Editado por Instituto de Ciencia y Tecnología de polímeros (CSIC), Madrid, 2004
- Macromoléculas (2 vol), A. Horta. 2ª reimpresión, Universidad Nacional de Educación a Distancia, Madrid, 2000
- Técnicas de caracterización de polímeros, M. A. Llorente, A. Horta. Universidad Nacional de Educación a Distancia, Madrid, Facultad de Ciencias, 1991
- Introducción a la química de los polímeros, R. B. Seymour, Charles E. Carraher. Reverté, Barcelona, 1995.
- Principles of polymerization, G. Odian. 3rd Ed., Wiley, New York, 1991
- Polymer synthesis and characterization: A laboratory manual, S. R. Sandler. Academic Press, San Diego 1998.

Other bibliographic works to consult

- Comprehensive Polymer Science: the Synthesis, Characterization, Reactions & Applications of Polymers, G. Allen. Pergamon Press, Oxford, 1989.
- Polymers: Chemistry and Physics of Modern Materials, J.M.G. Cowie. 2nd Ed., Stanley Thornes, Cheltenham, United Kingdom, 1998.
- New methods of polymer synthesis (2 vol), J. R. Ebdon. Blackie Academic & Professional, London 1995-1997
- Modern techniques for polymer characterization, R.A. Pethrick, J.V. Dawkins. John Wiley & Sons, Chichester, 1999
- Experimental methods in polymer science: Modern methods in polymer research and technology, T. Tanaka. Academic Press, San Diego 2000.

INTERNET RESOURCES

http://www.ubu.es/biblioteca/resources_inet/estadistica_m.htm
http://www.polymersdatabase.com/

ASSESSMENT

Methodology

- Preparation and presentation of reports
- Preparation of assignments
- Resolution of exercises and practical cases
- Participation in seminars, tutorials and other activities
- Completion of assessment tests
- Final Exam

Marking criteria

- Preparation and presentation of reports 40%

-	Resolution of exercises and practical cases	15 %
-	Participation in seminars, tutorials and other activities	15 %
-	Completion of assessment tests	30 % (3 tests)

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1.-	Félix García	12	12
Unit 2.-	José Luis de la Peña	10	10
Unit 3.-	José Miguel García	13	12
Unit 4.-	José Miguel García	10	10
Activities	Félix García / José Miguel García	10	6
Exam preparation.		--	15
Completion of final assessment test		5	--
Total	**125**		

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
ADVANCED METHODS IN EXPERIMENTAL DESIGN AND NATURAL COMPUTATION			5250
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	2	Semi-optional	5 (3T/2P)

LECTURER (1) IN CHARGE OF THE COURSE			
Luis Antonio Sarabia Peinador			
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LECTURER (2)			
María Cruz Ortiz Fernández			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Analytical Chemistry
Office	Tel. num. (Ext.)	Email	
	947-258800 (8211)	mcortiz@ubu.es	

LECTURER (3)			
Mª Sagrario Sánchez Pastor			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Mathematics and Computation	Area	Statistics and operational Research
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	947-258829	ssanchez@ubu.es	

LECTURER (4)

Ana Herrero Gutiérrez			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Analytical Chemistry
Office	Tel. num. (Ext.)	Email	
	947-258800 (8211)	aherrero@ubu.es	

STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures		15
	Attendance at practical classes (laboratory or computer room)		30
	Attendance at seminars and activities		5
	Attendance at assisted tutorials		5
	Presentation of assignments		2
	Completion of assessment tests		3
PRIVATE STUDY	Group work for theoretical and/or practical classes.		15
	Study for the preparation of theoretical and/or practical classes.		25
	Resolution of exercises and practical cases, preparation of reports and presentations		15
	Exam preparation.		10
Total hours (Taught Classes)	60	**Total hours (Private Study)**	65
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

Factor selection. Interpretation. Optimization based on response surface models. Experimental design quality. Mixtures. Made-to-measure designs. Estimates and decisions based on computer-intensive methods. Evolutionary algorithms. Neural networks. Methods for filtering signals.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

It is recommended that students possess: a basic knowledge of basic statistics and procedures in analytical chemistry and instrumental chemical techniques.

OBJECTIVES

General

- To understand the need for an experimental methodology.
- To understand the advantages of reducing mathematical hypotheses for the construction of models.
- To understand and operate experimental design tools for the articulation and resolution of problems in scientific research and industrial applications.
- To gain familiarity with certain specific applications for experimental design and natural computation.

- To understand the difference between analytical and computational methods, their basis and their potential applications.

Specific

- To advance a satisfactory model for each experimental design that explains the functional relations between factors and responses.
- To perform the relevant experimental plan in each case under study.
- To analyse the significance of experimental factors in the area under analysis.
- To detect and quantify the influence of factors in one or various experimental responses.
- To optimize response surfaces.
- To know how to use efficient designs. To use sequentiality.
- To use desirability functions in the context of chemical analysis, in a process and in the manufacture of the product.
- To apply optimization in mixture problems with and without constraints.
- To construct experimental designs based on D-optimality and other properties.
- To understand and conduct supersaturated designs.
- To perform numerical optimisation.
- To filter signals in order to improve the signal/noise relation.
- To optimize without a functional model through genetic algorithms.
- To construct, train and validate neural networks.
- To calculate estimators and use them as a basis for decisions.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

The course will enable the student to:

Knowledge

- Understand experimental design methodology
- Become familiar with "standard" experimental design and its adaptation to problem types
- Become familiar with the existence of alternative computer-based methods and their basis
- Understand the concept of a neural network and its training.
- Understand the basis of genetic algorithms.

Skills

- Propose solutions to problems in the same terms as they are expressed.
- Implement different technical aspects in the field of work.
- Evaluate, interpret and summarise chemistry-related data and information.
- Implement good practice in scientific measurement and experimentation.

- Operate specific software.
- Optimise analytical procedures, processes and products
- Take objective decisions under uncertainty conditions
- Plan, design and execute (develop) practical research from the recognition of a problem up until the evaluation of its results.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Deductive reasoning skills and the application of creative thinking, through their introduction into applied research.
- Analytical and summary skills.
- Ability to organise and to adapt to new situations.
- Report preparation and presentation skills.
- Oral and written communication skills in the student's 1st language.
- User knowledge of computing tools and information technology.
- Skills involving the application of theoretical knowledge in practical work.
- Aptitude for autonomous learning and self-study.
- Ability to search for and retrieve information, from both primary and secondary sources, including information obtained through on-line communication and by accessing data banks.
- Integration into work groups, above all interdisciplinary ones.
- Motivated by quality
- Critical reasoning and capacity for self-evaluation.
- Problem-solving skills relating to qualitative and quantitative information.

STUDY PLAN

Unit 1. Experimental design methodology
Mathematical design model. Experimental matrix. Experimental plan. Model validation. Effects. Factors: Experimental plan. Criteria: Orthogonal design, D-optimal, E-optimal, and G-optimal designs, rotatables, etc. Inflation and variance factors. Design classification by its final purpose.

Unit 2. Designs for the selection of factors.
Hadamard designs and highly fractional designs for the selection of factors. Estimation of the replicated and unreplicated residual variance (the Lenth method). Fractional designs at various levels: Presence/absence models, reference state models. Supersaturated designs. Application to the study of chemical interferences. Applications to the robustness of analytical procedures.

Unit 3. Factorial designs.
Factorial designs at two or more levels. Experimental plans. Calculation of the effects of the principal factors and the interactions. Fractional designs. Confusion patterns. Generators. Drift levels. Blocking. Environmental factors (Taguchi designs). Industrial and analytical applications.

Unit 4. Designs for response surface.
The search for optimal levels through representation of the response surface with two-factor designs. Central composite designs, pentagonal and hexagonal designs, etc. Sequentiality with Doehlert designs. Blocking. Optimization with more than two factors. Canonical form. The optimal path method. Optimization of the instrumental signal, of an extraction, of a synthesis. Desirability function (Derringer). Applications to the optimization of the signal and diminishment of the variance in chemical analysis.

Unit 5. Designs for surface responses.
Mixture diagrams. Linear and quadratic models. Scheffé designs. Calculation of coefficients by least squares. Experimental plans for the optimization of mixtures with and without constraints. Mixture problems in industrial and food products and in the laboratory (eluents in chromatography).

Unit 6. Non-standard designs.
Need for these designs because of restriction problems in the experimental domain. Designs based on D-optimality. Mathematical models. Candidate points. Exchange algorithms. Applications in problems with high experimental costs. Specific designs for computer simulations. Applications in the automotive industry, the energy sector, etc.

Unit 7. Sequential optimization
Optimization with linear models. Maximum slope method. Optimization without a mathematical model: SIMPLEX. On-line optimization. Operational evolution method.

Unit 8. Computer-intensive techniques
Methods of estimation and decision making using Monte Carlo, bootstrap, etc. Optimization using genetic algorithms. Non-parametric models based on neural networks.

Unit 9. Smoothing and filtering of signals
Smoothing a local polynomial. The Savitzky-Golay method. Spline differentiation. Fourier-transform smoothing.

METHODOLOGY

The subject is developed by interspersing fundamental theoretical and practical knowledge needed to resolve problems, through the use of specific professional software for the set objectives (NemrodW, Matlab) and by making use of real data that define the case studies.

Once the fundamental theoretical aspects are understood and having confirmed that they have been correctly applied to the resolution of the set problem, an open debate is held on the results and the conclusions that are reached, and the next steps to take, if the problem so requires. This sequence of activities will enable students to progress through the construction and internalisation of their own knowledge of the subject matter.

They will obtain experimental data in the chemical analysis laboratory or in industry through appropriate experimental designs and interpret and evaluate the results through individual written reports defended in front of the other students.

BIBLIOGRAPHY

Basic reference works

Montgomery, D.C., Design and analysis of experiments, Fourth edition, John Wiley & Sons. 1997

Myers, R.H., Montgomery, D.C., Response surface methodology. Process and product optimization using designed experiments, John Wiley & Sons 1995, New York.

Lewis, G.A. Mathieu, D. Phan-Tan-Luu, R., Pharmaceutical Experimental Design, Drugs and Pharmaceutical Sciences, vol. 92, Marcel Dekker, Inc., 1999

Box, G.E.P., Draper, N.R., Empirical model-building and response surfaces, John Wiley & Sons, Inc., 1987

Cornell, J.A., Experiments with mixtures, John Wiley & Sons, Inc., 1990

Michalewicz, Z. Genetic Algorithms + Data Structures = Evolution Programs, Springer, Berlin, 1996.

Bishop, C.M., Neural networks for pattern recognition, Oxford University Press: Clarendon Press, 1997

Bracewell R.N., The Fourier transform and its applications, McGraw-Hill International Editions, 1986.

Other bibliographic works to consult

Fogel, D.B. Evolutionary Computation: Toward a New Philosophy of Machine Intelligence, IEEE Press, Piscataway (NJ), 1995.

Holland, J.H. Adaptation in Natural and Artificial Systems, 2nd ed., MIT Press, Cambridge (MA), 1992.

Davis, L. (Ed.) Handbook of Genetic Algorithms, Van Nostrand Reinhold, New York (NY), 1991.

Goldberg, D.E. Genetic Algorithms in Search, Optimization and Machine Learning, Addison-Wesley, Reading (MA), 1989

T. Hastie, R. Tibshirani, J. Friedman, The elements of Statistical learning. Data mining, Inference, and Prediction, Springer Series in Statistics, Springer, 2001.

B.D.Ripley, Pattern recognition and neural networks, Cambridge University Press, 1996.

K. Deb, Multi-Objective optimization using evolutionary algorithms, Wiley, 2001

W.L. Martinez, A.R. Martinez, Computational Statistics Handbook with MATLAB, Chapman

and Hall/CRC, 2002, accessible at
http://www.ubu.es/biblioteca/recursos_inet/estadistica.htm
http://www.lania.mx/~ccoello/EMOO/EMOObib.html
Practical Handbook of Genetic Algorithms, Lance Chambers (ed.), CRC Press, 1995
Applications of Multi-Objective Evolutionary Algorithms, Carlos A Coello Coello, Gary B Lamont (eds), World Scientific, 2005

INTERNET RESOURCES

http://www.statsoft.com/products/doe.html
http://www.systemtechnik.tu-ilmenau.de/~pohlheim/EA_Matlab/ea_matlab.html
http://www.aic.nrl.navy.mil/galist/
http://www.cs.uwyo.edu/~wspears/functs.html
http://www.geatbx.com/
http://panizzi.shef.ac.uk/cisrg/links/ea_bib.html
http://www.isixsigma.com/dictionary/Design_of_Experiments_-_DOE-41.htm
http://www.wtec.org/loyola/welcome.htm

ASSESSMENT

Methodology

- Preparation and presentation of reports
- Preparation of assignments
- Resolution of exercises and practical cases
- Participation in seminars, tutorials and other activities
- Completion of a individual assessment test at the end of the course

Marking criteria

- Preparation and presentation of reports: 20%
- Preparation of assignments: 20%
- Resolution of exercises and practical cases: 20%
- Participation in seminars, tutorials and other activities: 15%
- Completion of a individual assessment test at the end of the course: 25%

PROGRAMMED ACTIVITIES (Subject matter and Study hours)

Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1. Experimental design methodology	Luis A. Sarabia Ana Herrero Mª Cruz Ortiz Mª Sagrario Sánchez	1	2
Unit 2. Designs for the selection of factors.		5	4
Unit 3. Factorial designs.		9	8
Unit 4. Designs for response surface.		15	15
Unit 5. Designs for mixtures.		6	5
Unit 6.Non-standard designs		6	6
Unit 7. Sequential optimization		5	5
Unit 8. Computer-intensive techniques		5	5
Unit 9. Smoothing and filtering of signals		5	5
Exam preparation.		--	10

Completion of final exam		3	--
Total	125		

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
ADVANCED ELECTROCHEMICAL METHODS			5247
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (4/1)

LECTURER (1) IN CHARGE OF THE COURSE			
Jesús López Palacios			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Analytical Chemistry
Office	Tel. num. (Ext.)	Email	
Q.A. 20 (199)	947 25 88 17	jlopal@ubu.es	

LECTURER (2)			
Mª Julia Arcos Martínez			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Analytical Chemistry
Office	Tel. num. (Ext.)	Email	
Q.A. 19 (198)	947 25 88 18	jarcos@ubu.es	

STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	2	30
	Attendance at practical classes (laboratory or computer room)	1.6	24
	Attendance at seminars and activities	--	--
	Attendance at assisted tutorials	0.8	12
	Presentation of assignments	0.3	5
	Completion of assessment tests	--	4
PRIVATE STUDY	Group work for theoretical and/or practical classes.	--	--
	Study for the preparation of theoretical and/or practical classes.	0.7	10
	Resolution of exercises and practical cases, preparation of reports and presentations	1.3	20
	Exam preparation.	1.3	20

Total hours (Taught Classes)	75	**Total hours (Private Study)**	50
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

The study of advanced electrochemical technology: spectroelectrochemistry, sensors, electrochemical microscopy, electrochemical quartz crystal microbalance, electrochemical impedance.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

- ✓ It is recommended that the student possess a basic knowledge of electrochemistry.

OBJECTIVES

General

- ✓ To understand the basis and the characteristics of the electrochemical methods that are presented, studying their possible application in different industrial land research fields.

Specific

- ✓ To understand the fundamentals of mixed instrumental techniques based on electrochemistry.
- ✓ To study different configurations in spectroelectrochemical systems.
- ✓ To analyze the potential of quartz crystal microbalance as an electroanalytical tool.
- ✓ To acquire a basic knowledge of scanning electrochemical microscopy (SEM).
- ✓ To understand the theoretical basis of electrochemical impedance.
- ✓ To gain awareness of the potential of modified electrodes in the analysis of substances of biological interest.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

The course will enable the student to:

- ✓ Analyse complex electrochemical signals.
- ✓ Understand instrumental schemes.
- ✓ Gain skills at capturing diverse signals produced simultaneously in a chemical process.

- ✓ Analyse electrochemical devices on micro- and nanometric scale.
- ✓ Construct modified electrodes for various applications.
- ✓ Manipulate enzymes.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- ✓ Deductive and predictive-reasoning skills.
- ✓ Ability to acquire knowledge for the interpretation of actual phenomena.
- ✓ Ability to relate phenomena and theories of a different nature.
- ✓ Critical and detailed process analysis skills.
- ✓ Abilities to research and process information.
- ✓ Formal preparation and description of models.
- ✓ Oral and written communication of complex phenomena.

STUDY PLAN

Unit 1. Spectroelectrochemistry
Fundamentals. Standard transmission cells: Optically transparent electrodes. Parallel transmission: long-optical-path cells. Bidimensional Spectroelectrochemistry Reflection cells. Flow systems. Examples of applications.

Unit 2. The electrochemical crystal quartz microbalance.
Piezoelectricity. The crystal quartz microbalance. The Sauerbrey equation. The quartz oscillator electromechanical model: the Butterworth-van Dyke model. The quartz microbalance in electrochemical experiments.

Unit 3. Scanning electrochemical microscopy (SECM).
Electrochemical responses in macro- and microelectrodes: Fundamentals of electrochemical microscopy. SECM operating modes. Amperometric feedback responses: positive and negative feedback. Sweep mode: obtaining images. Applications.

Unit 4. Electrochemical impedance.
Alternative current in electrochemistry: responses in potential and current through resistances, capacitances and inductances. Resistance-capacitance (RC) circuits. The concept of impedance. The equivalent circuit of an electrochemical cell. Resistance, capacitances and inductances in electrochemical cells. Warburg electrochemical impedance. Measurement techniques. Graphic methods in the analysis of impedances: Nyquist, Bode and Randles diagrams. Some practical cases.

Unit 5. Modified electrodes.
Carbon-paste electrodes. Polymeric electrodes. Polymer conductors: Enzymatic electrodes.

Unit 6. Biosensors.
Substrates. Immobilization methods. Transductors. 1st generation biosensors. 2nd generation biosensors. 1st generation biosensors. Applications.

METHODOLOGY

- ✓ Theoretical classes supported by computer mediums.
- ✓ Analysis and open discussion of the themes, with the active participation of students.
- ✓ Practical classes with the instrumentation available in the Department.
- ✓ Preparation of personal and group work on advanced research themes.
- ✓ Guided searches for information using information technology.

BIBLIOGRAPHY

Basic reference works

- ✓ A.J. Bard and L.R. Faulkner, Electrochemical Methods, Wiley, 2000
- ✓ P.H. Rieger, Electrochemistry, Prentice-Hall, 1987 (Cap. 5)
- ✓ C.M.A. Brett and A.M.O. Brett, Electrochemistry. Principles, methods and applications, Oxford Science Publications, 2003 (Caps. 4-6)
- ✓ G. Inzelt, Kinetics of Electrochemical Reactions, en Electroanalytical Methods, (F. Scholz Ed.), Springer, 2002. (Parte I, cap. 3)
- ✓ P.T. Kissinger, C.R. Preddy, R.E. Shoup and W.R. Heineman, Fundamental Concepts of Analytical Electrochemistry, en Laboratory Techniques in Electroanalytical Chemistry, (P.T. Kissinger and W.E. Rubistein Ed., Marcel Dekker, 1984.

Other bibliographic works to consult

- ✓ Rubinstein, Fundamentals of Physical Electrochemistry, en Physical Electrochemistry (I. Rubinstein, Ed.), Marcel Dekker, 1995.
- ✓ M. Sluyters-Rehbach, Impedances of electrochemical systems, Pure & Applied Chemistry 66 , 9, (1994), 1831-1891.

INTERNET RESOURCES

http://www.consultrsr.com/
http://wwwecochemie.nl
http://www.princetonappliedresearch.com/
http://www.princetonappliedresearch.com/products/appnotes.cfm

ASSESSMENT

Methodology

- Continuous evaluation of the active participation of students during the taught classes.
- Preparation and presentation of individual or group reports (according to student numbers on the course).
- Written assessment tests

Marking criteria

- ✓ Written assessment tests 30%
- ✓ Preparation and presentation of assignments: 40%
- ✓ Written exam: 50%

PROGRAMMED ACTIVITIES (Subject matter and Study hours)

Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1.- Espectroelectrochemistry	Jesús López Palacios	5	1

Unit 2.- The electrochemical crystal quartz microbalance.	Jesús López Palacios	5	1
Unit 3.- Scanning electrochemical microscopy.	Jesús López Palacios	5	1
Unit 4.- Electrochemical impedance.	Jesús López Palacios	5	1
Unit 5.- Modified electrodes.	Julia Arcos Martínez	5	1
Unit 6.- Biosensors.	Julia Arcos Martínez	5	1
Laboratory practicals	Jesús López Palacios/ Julia Arcos Martínez	24	4
Preparation and presentation of assignments	Jesús López Palacios/ Julia Arcos Martínez	5	20
Tutorials for the preparation of assignments	Jesús López Palacios/ Julia Arcos Martínez	12	--
Exam preparation.		--	20
Completion of final assessment test	Jesús López Palacios/ Julia Arcos Martínez	4	--
Total hours		**125**	

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			**CODE**
MODERN METHODS OF ORGANIC SYNTHESIS			5248
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (4/1)

LECTURER (1) IN CHARGE OF THE COURSE			
Tomás Torroba Pérez			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
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LECTURER (2)			
Roberto Sanz Diez			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Organic Chemistry
Office	Tel. num. (Ext.)	Email	
1B08	947 258036	rsd@ubu.es	

LECTURER (3)			
María García Valverde			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Organic Chemistry
Office	Tel. num. (Ext.)	Email	
1B06	947 259529	magaval@ubu.es	

STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	2.5	39
	Attendance at practical classes (laboratory or computer room)	1.6	24
	Attendance at seminars and activities	0.2	3
	Attendance at assisted tutorials	0.2	3
	Presentation of assignments	0.2	3
	Completion of assessment tests	0.2	3
PRIVATE STUDY	Group work for theoretical and/or practical classes.	0.3	5
	Study for the preparation of theoretical and/or practical classes.	0.7	10
	Resolution of exercises and practical cases, preparation of reports and presentations	1.7	25
	Exam preparation.	0.7	10

Total hours (Taught Classes)	75	**Total hours (Private Study)**	50
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

Multicomponent and tandem reactions. Diversity oriented synthesis. Organometallic reagents in Organic Synthesis. Transition metal organometallic compounds. Asymmetric synthesis. Synthesis selectivity. Stereochemistry of reactions.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

Knowledge of organic, inorganic, physical and analytical chemistry at graduate level.
Knowledge of physics at graduate level.

Objectives

General

- To introduce the student to some of the more powerful techniques of organic synthesis that will be useful at the research stage.
- To present to the student the enormous difference between classic organic synthesis reactions, in which two reagents react to produce a product, and reactions in which a range of components react sequentially to arrive at a product that is the sum of those same successive reactions.
- To impart knowledge on new synthetic methods based on the use of organometallic compounds.
- To bring to the fore the importance of organometallic chemistry as a field that links organic and inorganic chemistry.
- To introduce the student to the creation of complexity in the synthesis of heterocycles.
- To introduce the student to basic synthetic techniques for small molecule libraries.
- To demonstrate the importance of stereochemical control in the development of organic reactions.

Specific

- To understand the reactivity of the principal groups of organometallic compounds, fundamentally, organolithium and organomagnesium compounds, as well as their principal applications in organic synthesis.

- To understand the synthetic potential that some complex transition metals present as catalysts in C-C bond forming reactions.
- To acquire an ability to manage multicomponent, tandem and domino reactions.
- To be able to combine known processes in the search for new synthetic processes.
- To be able to design complex products, especially heterocyclic ones, through the simultaneous application of multicomponent, tandem and domino reactions, and combined reaction acceleration techniques.
- To give the student the necessary tools to control and interpret, from a stereochemical perspective, the reactions that are produced in the laboratory.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

The course will enable the student to:

- Gain sufficient knowledge to approach the study of a new synthetic process that presents certain characteristics of complexity, specificity and stereoselectivity.
- To acquire, analyse and interpret specific data related to a new synthetic process and to combine it in a new design.
- To be conscious of the possibilities and limitations of a new synthetic process, as well as being able to use the most appropriate instrumental techniques to monitor its progress correctly.
- To understand the applications of new multicomponent and sequential applications in the synthesis of high value products, principally in the field of industry.
- To acquire abilities and systematic approaches in the synthesis and characterization of an organic compound in the laboratory through very selective organometallic processes.
- To be able to work in the laboratory in accordance to safety norms and to respect the environment.
- To be able to apply critical scientific methods to the theoretical and experimental study of new materials.
- To be able to prepare a technical report that may be understood by anybody that has received a scientific training but is not an expert in the subject.
- To be able to make an oral presentation and lead a group discussion on the results of a thermal, electrical, optical, photophysical or magnetic study.
- To acquire theoretical and experimental abilities that allow other more complex ones to be assimilated.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND SYSTEMATIC).

- Oral and written communication skills in the student's first language
- Ability to research and obtain information.
- Ability to analyse, summarise, prepare and present reports.
- Problem-solving skills relating to qualitative and quantitative information.
- Ability to apply the theoretical knowledge acquired.
- Abilities and skills in all practical aspects relating to laboratory work.
- Study skills and autonomous learning skills, necessary for ongoing training and professional development
- Skills related to computer tools and information technology.
- Interpersonal skills, appropriate for interpersonal relations and for integration in work groups.
- Decision-making capacity
- Ability to integrate quality as one of the most important variables to consider.
- Deductive reasoning skills and the ability to exploit creative thinking through its introduction into research.

– Ability to recognise aspects related to occupational safety and environmental impact as fundamental aspects of the student's professional conduct.

STUDY PROGRAMME

Unit 1: Multicomponent and Tandem Reactions, Diversity-Oriented Synthesis

1.1. An overview of multicomponent reactions in Organic Synthesis.
- 1.1.a. Three-component reactions. Petasis-Mannich, Bailys-Hillmann.
- 1.1.b. Isocyanide multicomponent reactions. New processes - Passerini, Ugi.
- 1.1.c. Multicomponent reactions in heterocyclic synthesis.
- 1.1.d. Tandem and domino reactions or cascade processes.
- 1.1.e. Applications of tandem and domino reactions in heterocyclic synthesis.

1.2. Diversity-oriented synthesis.
- 1.2.a. Solid-phase combinatorial chemistry.
- 1.2.b. Combinatorial chemistry solutions.
- 1.2.c. Obtaining structural complexity in organic synthesis.

Laboratory experiments: Preparation of compounds of pharmacological interest through multicomponent and sequential reactions.

Unit 2: "Organometallic reactives in Organic Synthesis."

2.1. Organometallic compounds of the Main Groups
- 2.1.a. Organolithium and organomagnesium compounds
- 2.1.b. Organometallic compounds of zinc

2.2. Transition Metal Organometallic Compounds.
- 2.2.a. Organocuprates
- 2.2.b. Zirconium and titanium
- 2.2.c. C-C bond forming reactions catalysed by Pd and Ni complexes

Laboratory experiments: Synthesis of compounds of interest through the use of organometallic reagents.

Unit 3: Asymmetric synthesis

3.1: Selectivity in Organic Synthesis.
- 3.1.a. Stereochemical vocabulary
- 3.1.b. Methods to determine enantiomeric purity
- 3.1.c. Methods to Obtain Chiral Compounds
- 3.1.d. Energetic Considerations
- 3.1.e. Stereoelectronic effects. Frontier Molecular Orbital (FMO) theory

3.2. The Stereochemistry of Reactions.
- 3.2.a. Bimolecular Nucleophilic Substitution
- 3.2.b. Additions to Carbonyl Compounds
- 3.2.c. Enolate reactions.
- 3.2.d. Additions to C-C Double Bonds
- 3.2.e. Cycloadditions and Electrocyclic Reactions
- 3.2.f. Rearrangements

Laboratory experiments: Preparation of chiral compounds by stereoselective methods.

METHODOLOGY

- Lectures in which the fundamental aspects, objectives and working methods for each unit of the course are set out.
- Development of the work in three stages: (i) fundamental aspects of the sequence of reactions under study; (ii) case-by-case study; (iii) application to practical problems and examples.
- Organisation of participative seminars in which students become familiar with the theoretical content of the course.

- Interdisciplinary laboratory work on different stages of knowledge.
- Individual selection of a topic and preparation of an assignment on the same subject guided by the course lecturers.

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Basic reference works

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11. I. Ugi, A. Dömling: "Multi-component reactions (MCRs) of isocyanides and their chemical libraries", in: "Combinatorial Chemistry" H. Fenniri (Hrsg.), a.d.R.: "Practical Approach", Oxford University Press, Oxford 2000, p. 287-302
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15. T. Torroba: Poly-Sulfur-Nitrogen Heterocycles via Sulfur Chlorides and Nitrogen Reagents, J. Prakt. Chem. 1999, 341, 99-113.
16. "Organolithiums: Selectivity for Synthesis"; J. Clayden; Pergamon: Oxford, 2002
17. "Organomagnesium Methods in Organic Synthesis"; B.J. Wakefield; Academic Press: S. Diego, 1995
18. "Applications of Transition Metals Catalysts in Organic Synthesis"; L. Brandsma, S.F. Vasilevsky, H.D. Verkruijsse; Springer-Verlag: Berlin, 1998
19. -"Titanium and Zirconium in Organic Synthesis"; Ed.: I. Marek; Wiley-VCH: Weinheim, 2002
20. -"Metal-Catalyzed Cross-Coupling Reactions"; Eds.: F. Diederich, P.J. Stang; Wiley-VCH: Weinheim, 1998
21. -"Basic Organic Stereochemistry"; Eliel, E. L.; Wilen, S. H.; Doyle, M. P.; Wiley, 2001.
22. -"Principles and Applications of Asymmetric Synthesis"; Lin, G.-Q.; Li, Y.-M.; Chan, A.S.C.; Wiley, 2001.

Other bibliographic works to consult

1. Nicolaou, K. C.; Hanko, R.; Hartwig, W.: Handbook of Combinatorial Chemistry; Wiley-VCH: Weinheim, 2002; Vols. 1 and 2.
2. Eric M. Gordon, James F. Kerwin: Combinatorial Chemistry and Molecular Diversity in Drug Discovery, Wiley, New York, August 1998.
3. Prakash GKS, Mandal M, Schweizer S, Petasis NA, Olah GA: Stereoselective synthesis of anti-alpha-(difluoromethyl)-beta-amino alcohols by boronic acid based three-component condensation. Stereoselective preparation of (2S,3R)-difluorothreonine, J. Org. Chem., 2002, 67, 3718-3723.
4. "Organometallics in Synthesis: A Manual"; Ed.: M. Schlosser; Wiley: Chichester, 2002.
5. Handbook of Organopalladium Chemistry"; Ed.: E. Negishi; Wiley: New York, 2002
6. "Stereoselectivity in Organic Synthesis"; Procter, G.; Oxford Press University, 1998.
7. "Frontiers Orbitals and Organic Chemical Reactions", Felming, I.; Wiley, 1976.
8. "Catalytic Asymmetric Synthesis" Ed. Ojima, I.; Wiley, 2000.

INTERNET RESOURCES

ISI Web of Knowledge
http://www-g.eng.cam.ac.uk/photonics/blcs/
http://www.ch.ic.ac.uk/vchemlib/
http://www.ch.ic.ac.uk/vchemlab/symmetry/

http://www.chemie.uni-regensburg.de/external.html
http://www.chem.ucla.edu/chempointers.html
http://www.library.ucsb.edu/subjects/chem/chemistr.html
http://www.shef.ac.uk/~chem/chemdex/
http://www.anachem.umu.se/eks/pointers.htm
http://www.umass.edu/microbio/rasmol/scripts.htm#chime
http://chemfinder.cambridgesoft.com/
http://www.jce.divched.org/JCEDLib/QBank/collection/ConcepTests/
http://www.ch.cam.ac.uk/resources/

ASSESSMENT

Methodology

- Continuous assessment of training and learning outcomes evaluating each student's progress on the basis of:
  - f) The solution of exercises and practical cases
  - g) Participation in seminars, tutorials
  - h) Laboratory work.
  - i) Preparation and presentation of reports
  - j) Preparation, presentation and defence of an individual assignment.
- Final assessment: A final written test will be set on all the subject matter.

Marking criteria

Continuous evaluation. 40%
This mark represents an evaluation of the active participation of the student, the answers given to the theoretical-practical cases that are set, the development of laboratory work and, where applicable, the preparation and presentation of reports.

Final exam 30%
A four-hour final written exam on all of the subject matter, consisting of responses to questions and selected problems.

Preparation, presentation of an assignment. 30%

Each student will prepare a written assignment, which must be presented in public (for 30 minutes) and defended in front of the course lecturers. The subject matter must be chosen from among those put forward by the lecturers.

PROGRAMMED ACTIVITIES (Subject matter and Study hours)

Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1.-: Multicomponent and Tandem Reactions, Diversity-Oriented Synthesis	Tomás Torroba Pérez	24	14
Unit 2.-: Organometallic Reagents in Organic Synthesis.	Roberto Sanz Diez	24	13
Unit 3.-: Asymmetrical synthesis	María García Valverde	24	13
Exam preparation.		--	10
Completion of final assessment test		3	--
Total		**125**	

	MASTER's DEGREE IN ADVANCED CHEMISTRY **POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY** **DEPARTMENT OF CHEMISTRY** **FACULTY OF SCIENCES** **UNIVERSITY OF BURGOS.**

COURSE			CODE
CHEMIOMETRIC MULTIVARIATE AND MULTIVARIANT METHODS			5251
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (3T/2P)

LECTURER (1) IN CHARGE OF THE COURSE			
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Mª Sagrario Sánchez Pastor

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STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	15/15	15
	Attendance at practical classes (laboratory or computer room)	30/15	30
	Attendance at seminars and activities	5/15	5
	Attendance at assisted tutorials	5/15	5
	Presentation of assignments	2/	2
	Completion of assessment tests	3/	3
PRIVATE STUDY	Group work for theoretical and/or practical classes.	15/15	15
	Study for the preparation of theoretical and/or practical classes.	25/15	25
	Resolution of exercises and practical cases, preparation of reports and presentations	15/15	15
	Exam preparation.	10/15	10
Total hours (Taught Classes)	60	**Total hours (Private Study)**	65
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

Chemistry information. Recognition of patterns. Description of multivariate experimental data. Classification and modelling of categories. Relations between multiple variables and one or various responses. Quantitative possibilities of hyphenated instrumentation. Multivariate calibrations for multiway techniques.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

Knowledge of basic statistics. Knowledge of procedures in analytical chemistry and instrumental techniques.

OBJECTIVES

General

- To understand the fundamental aspects of multiway regression methods.
- To construct models with predictive characteristics.
- To consider the role of cluster analysis in the generation of a working hypothesis.
- To understand the difference between a classification method and a modelling method.
- To evaluate the cases in which multi-way methods can be of use.
- To identify existing methods.
- To gain familiarity with a number of concrete applications.
- To express uncertainty of measurement

Specific
– To characterise categories through pattern recognition techniques applied to multivariate data. – To evaluate the sensitivity and the specificity of class models. – To be able to select appropriate calibration techniques for each particular analytical problem. – To learn how to apply regression techniques and to interpret the results. – To examine the quantitative possibilities of hyphenated instrumentation by means of multi-way calibration. – To deal with the possibilities of 1st of 2nd-order signals for analytical determination in the presence of unknown interferents. – To deal with the possibilities of either 1st or 2nd or higher order signals for process-oriented analytical techniques.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)
Knowledge (Understanding) – Understanding of information relevant to chemical instrumentation. – Detection-related skills and familiarity with multivariate models. – Multivariate statistical methods. – Principles and procedures employed in chemical analysis for the quantification of chemical compounds. Skills (Know how) – Contribute a solution to a problem in the same terms as it is expressed. – Implement different technical aspects in the field of work. – Evaluate, interpret and summarise chemistry-related data and information. – Ability to implement good practice in scientific measurement and experimentation. – Operate specific software packages. – Process data in relation to chemical information and models. – Take objective decisions under uncertainty conditions. – Plan, design and execute (develop) practical research from the recognition of a problem up until the evaluation of its results.
GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).
– Deductive reasoning skills and the application of creative thinking through its introduction in applied research. – Analytical skills and an ability to summarise. – Ability to organise and to adapt to new situations. – Report preparation and presentation skills. – Oral and written communication skills in the student's 1st language. – User knowledge of computing tools and information technology. – Skills involving the application of theoretical knowledge in practical work. – Aptitude for autonomous learning and self-study. – Ability to search for and retrieve information, whether from primary or secondary sources, including information obtained through on-line communication and through access to data banks. – Integration into work groups, above all interdisciplinary ones. – Critical reasoning and capacity for self-evaluation. – Problem-solving skills relating to qualitative and quantitative information.

STUDY PROGRAMME

Unit 1. Pattern Recognition Levels
Exploratory multivariate techniques. Analysis of hierarchic and non-hierarchic clustering. Principal components analysis. Correspondence Analysis. Biplot techniques: The interpretability of latent variables.
Unit 2. Multivariate classification
Techniques based on multivariate normality (Linear Discriminant Analysis - LDA, Quadratic Discriminant Analysis - QDA). Non-parametric alternatives. K-Nearest Neighbours method (KNN) and Classification and Regression Trees (CART).
Unit 3. Modelling techniques
Modelling based on multivariate normality (Unequal Dispersed Classes - UNEQ) and based on principal components (Soft Independent Modelling of Class Analogies - SIMCA). Modelling power and discriminating power of variables. Sensitivity and specificity of models. Applications in the environmental and agroalimentary fields.
Unit 4. Regression techniques
Least-squares linear regression models. Outlier data and robust regressions. Prediction with regression models. Variable selection. Confidence in predictions. Alternating Conditional Expectation (ACE) regression. Colinearities and correlations between variables - some alternatives: Stepwise regressions based on latent variables.
Unit 5. Instrument calibration applications
The order of the signal. Two-way methods. Soft calibrations based on principal components. Partial-least-squares (PLS) calibrations. Its application to data taken from spectroscopic techniques: Near-Infrared Spectroscopy (NIR) and Mid-Infrared (MIR) Spectroscopy, ultraviolet-visible spectroscopy, molecular excitation and/or emission fluorescence, polarography, voltammetry, etc. Multi-way methods. N-way Partial Least Squares (N-PLS). Factorial decomposition by means of Parallel Factor Analysis (PARAFAC). Second-order advantage. PARAFAC2, TUCKER and other methodological possibilities. Applications to hyphenated instrumentation (CG-MS, HPLC-DAD, CL-MS-MS, flow techniques with electrochemical detectors), other techniques (molecular fluorescence excitation-emission).
Unit 6. Figures of merit with N-way calibrations
Multivariate analytical sensitivity. NAS. Detection capability with the evaluation of the probability of false positives and false negatives. Permitted limits in residues with evaluation of false non-conformities and false conformities.
Unit 7. Multivariate applications in industrial fields
Models for the typification of products and processes. Product classifications based on qualitative variables. Risk curves and evaluation of the probabilities of false non-compliant and false compliant with multivariate data. Regressions between process and product variables. Relations between physical-chemical variables and predictive sensory models using chemical and consumer-acceptance variables.

METHODOLOGY

The course work is developed by interposing the fundamental theoretical and practical knowledge that is necessary for the resolution of problems using specific professional software for the set objectives (PLS Toolbox in Matlab, STATGRAPHICS, PARVUS, PROGRESS and others). The concepts are introduced through the study of certain real cases and by obtaining, in the analytical laboratory, satisfactory experimental data for the problem in question. These data are used as practical examples so that the student may apply the methodology, prepare a report and defend it. Once the fundamental theoretical aspects are understood and having confirmed that they have been correctly applied to the resolution of the proposed problem, a shared debate follows on the results and conclusions obtained, and the next steps to take, if the problem so requires. This sequence of activities will enable students to progress through the construction and

internalisation of their own knowledge of the subject matter.

BIBLIOGRAPHY

Basic reference works

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N.R. Draper, H. Smith, Applied regression analysis, Second edition, Wiley series in probability and mathematical statistics, 1981.
H.Martens, T. Næs, Multivariate Calibration, John Wiley & Sons, Inc., 1989.
P.J. Rousseeuw, A.M. Leroy, Robust regression and outlier detection, John Wiley & Sons, 1987.
H.A. Kiers, A.K. Smilde, J. Chemom., 9 (1995) 179.
K.S. Books, Z. Lin, Z. Wang, B.R. Kowalski, Anal. Chem., 66 (1994) 2561.
Sánchez, E. Kowalski, B.R. J. Chemom., 29 (1990) 29.
Smilde, R. Bro, P. Geladi, Multi-way analysis, Wiley, Chichester, 2004.
T. Næs, T. Isaksson, T. Fearn, T. Davies, Multivariate Calibration and Classification, NIR Publications, Chichester, 2002.
R.G. Brereton, Chemometrics. Data analysis for the laboratory and chemical plant, Wiley, Chichester, 2003.
Massart, D.L, Vandeginste, B.G.M. Buydens, L.M.C. Jong, S. de Smeyeers-Verbeke, P.J. "Handbook of Chemometrics and Qualymetrics"; Part A and Part B in Data Handling in Science and Technology, Elsevier, Amsterdam, 1997.
K. Bakeev, Process Analytical Technology. Spectroscopic tools and implementation strategies for the chemical and pharmaceutical industries, Blackwell Publishing, 2005.
G. Saporta, Probabilités, analyse des donnés et statistique, Editions Technip, Paris, 1990.

Other bibliographic works to consult

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Brown P.J., "Measurement, Regression and Calibration" Claredon Press, Oxford, 1993.
J. H. Kalivas and P.M. Lang, "Mathematical Analysis of Spectral Orthogonality". Marcel Deckker, New York, 1994.
R. Cela, "Avances en Quimiometría Práctica", Servicio de publicaciones e Intercambio Científico. Campus Universitario de Santiago de Compostela, 1994.
R. Kellnel and others, "Analytical Chemistry: The approved text for the FECS curriculum analytical chemistry, Ed.Wiley-VCH, 1998.

INTERNET RESOURCES

http://www.models.kvl.dk/source/
http://www.eigenvector.com
http://www.spectroscopynow.com/coi/cda, (Chemometrics & Informatics tab)

ASSESSMENT

Methodology

- Preparation and presentation of reports.
- Preparation of assignments.
- Resolution of exercises and practical cases.

– Participation in seminars, tutorials and other activities. – Completion of a individual assessment test at the end of the course
Marking criteria
– Preparation and presentation of reports: 20% – Preparation of assignments: 20% – Resolution of exercises and practical cases: 20% – Participation in seminars, tutorials and other activities: 15% – Completion of a individual assessment test at the end of the course: 25%

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1. Pattern Recognition Levels.	Mª Cruz Ortiz Luis A. Sarabia Ana Herrero Mª Sagrario Sánchez	6	5
Unit 2. Multivariate classification.		6	5
Unit 3. Modelling techniques		6	5
Unit 4. Regression techniques		10	10
Unit 5. Instrument calibration applications		18	20
Unit 6. Figures of merit with N-way calibrations.		6	5
Unit 7. Multivariate applications in industrial fields		5	5
Exam preparation.		3	
Completion of final assessment test			10
Total		125	

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
DISSOLUTION PROCESSES: THE KINETICS AND THERMODYNAMICS OF COMPLEX REACTIONS			5256
Title	Centre		
Chemistry	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	2	Semi-optional	5 (4/1)

LECTURER (1) IN CHARGE OF THE COURSE			
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LECTURER (5)			
Saturnino Ibeas Cortés			
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STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	35/15	35
	Attendance at practical classes (laboratory or computer room)	1	15
	Attendance at seminars and activities	5/15	5
	Attendance at assisted tutorials	5/15	5
	Presentation of assignments	10/15	10
	Completion of assessment tests	5/15	5
PRIVATE STUDY	Group work for theoretical and/or practical classes.	5/15	5
	Study for the preparation of theoretical and/or practical classes.	10/15	10
	Resolution of exercises and practical cases, preparation of reports and presentations	10/15	5
	Exam preparation.	10/15	30
Total hours (Taught Classes)	75	**Total hours (Private Study)**	50
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

Conformation of biological macromolecules. Complexation reaction mechanisms with transition metals. The mechanisms of ADN-Ligand and Protein-Ligand intercalation reactions. Excess functions expressed in a polynomial form. Application of thermodynamics to biological processes. Advantages and limitations of homogeneous catalysis. Principal catalytic processes. Hydrogen and hydrogen transfer.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

Knowledge of chemistry, physics and mathematics at graduate level.

OBJECTIVES

General

To acquire and apply theoretical knowledge and methods to characterize complex reactions.

To understand different types of instrumental techniques and their application limits.
To enter into contact with the latest research in the field of reactions in dissolution.
To develop abilities to approach the resolution of scientific problems related to structural research and homogeneous catalysis.

Specific

- To understand protein and nucleic-acid structures.
- To understand the reaction mechanisms of proteins and nucleic acids with different types of ligands.
- To manipulate a number of instrumental techniques used in the determination of structural properties.
- To learn about theoretical and experimental methods related to the measurement of thermophysical properties.
- To study the advantages and limitations of homogeneous catalysis.
- To study different catalytic processes.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

- Safe handling of chemical materials.
- Principal aspects of chemical terminology, nomenclature, agreements and units.
- Types of chemical reactions and their principal associated characteristics.
- Recognition and analysis of new problems and planning strategies to solve them.
- Risk assessment in the use of chemical substances and laboratory procedures. Capacity to demonstrate knowledge and comprehension of essential facts, concepts, principals and theory related to areas of Chemistry.
- Ability to plan, design and execute practical research, from the problem-recognition stage up until the assessment and evaluation of the results and discoveries.
- Data interpretation skills derived from laboratory observation and measurement in terms of their signification and the theories that support them.
- Awareness of the possibilities and limitations and costs of biological material, as well as the most appropriate instrumental techniques for their characterization.
- Acquisition of abilities and systematic approaches to work relating to catalytic processes.
- Ability to conduct laboratory work in accordance with safety regulations and respect for the environment.
- Ability to apply critical scientific methods to the theoretical and experimental study of new materials.
- Ability to prepare a technical report that may be understood by anybody that is not an expert in the subject.
- Ability to make an oral presentation and lead a group discussion on the results of a theoretical or experimental study.
- Acquisition of theoretical and experimental skills that allow other more complex ones to be assimilated.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Oral and written communication skills in the student's 1st language.
- Ability to research and obtain information.
- Ability to analyse, to summarise, and to prepare and present reports.
- Problem-solving skills relating to qualitative and quantitative information.
- Ability to apply the theoretical knowledge acquired.
- Abilities and skills in all practical aspects related to laboratory work.
- Study skills and autonomous learning, necessary for ongoing training and

professional development.
- Skills related to computer tools and information technology. Interpersonal skills, appropriate for interpersonal relations and for integration in work groups.
- Decision-making skills.
- Ability to integrate quality as one of the most important variables to consider.
- Deductive reasoning skills and the ability to exploit creative thinking, through its introduction into research.
- Ability to recognise aspects related to occupational safety and environmental impact as fundamental aspects of professional conduct.

STUDY PROGRAMME

Unit 1: Conformation of biological macromolecules. Understanding the structure of proteins and nucleic acids.
Unit 2: Complexation reaction mechanisms with transition metals.
Unit 3: Mechanisms for ADN-ligand and protein-ligand intercalation reactions. Experimental techniques for the elucidation of reaction mechanisms.
Unit 4: Excess functions expressed in a polynomial form. Thermodynamic characterisation of symmetric, asymmetric, athermal and regular mixtures. Excess functions and mixability of the mixture. Theoretical dissolution models: van Laar, Hildebrand, Wohl.
Unit 5: Application of thermodynamics to biological processes. Polymeric dissolutions: Network models. The Flory-Huggins theory. The Prigogine-Flory-Paterson theory. Intrinsic viscosity and average molecular weight.
Unit 6: Advantages and limitations of homogeneous catalysis. Inorganic and organometallic complexes as catalysers. Metals and ligands in catalysis. Catalytic cycles. Elemental steps.
Unit 7: Principal processes. Isomerization. Carbonylation. Hydroformylation. Hydrocyanation and hydrosilylation. Oligomerization, polymerisation and olefin metathesis.
Unit 8: Laboratory practice related with units 1, 2 and 3

METHODOLOGY

- Lectures in which the foundation, objectives and working methods are set out for the contents of each subject area. Development of the work in three stages: (i) fundamental aspects of the properties under study; (ii) case by case study; (iii) application to practical problems and examples. Organisation of participative seminars in which students become familiar with the theoretical content of the course. Interdisciplinary laboratory work in different areas of knowledge. Preparation and presentation of laboratory reports. Individual selection of a topic and preparation of an assignment on the same subject guided by the subject lecturers.

BIBLIOGRAPHY

Basic reference works

C.R. Cantor, P. R. Schimmel, *Biophysical Chemistry,* W.H. Freeman and Company, New York, 1980.
C. Gómez-Moreno and J. Sancho Sanz, *Estrucutura de Proteinas,* Ariel Ciencia, 2003.
Van Ness H. C., Smith J. M. and Abbot M. M., *Introducción a la Termodinámica en la Ingeniería Química.* McGraw-Hill, 1997.
Assel M. J., Trusler J. P. M and Tsolakis T. F., *Thermophysical Properties of Fluids*. Ed. Imperial Collage Press, 1998.

Prausnitz, J. M., Lichtenthaler R. N. and Gomes de Acebo E., *Termodinámica Molecular de los equilibrios de fases*. Prentice Hall, 2001.
Muriel J. N., and Jenkins A. D., *Properties of Liquids and Solutions,* Second Edition, John Wiley & Sons, 1997.
Bevan Ott J. and Boerio-Goates J., *Chemicals Thermodynamics. Advanced Applications*. Academic Press, van Leeuwen, P.W.N.M., Kluwer, *Homogeneous Catalysis,* 2004.
Gates, B. C. *Catalytic Chemistry,* Wiley, 1992.
C.M. Starks, C.L. Liotta, M. Halpern, *Phase Transfer Catalysis,* Chapman & Hall, 1994.
J. Reedijk, E. Bouwman. *Bioinorganic Catalysis*, Marcel Dekker, 1999.

Other bibliographic works to consult

- E.F.Caldin *The Mechanism of Fast Reaction in Solution*, IOS Press, 2001

INTERNET RESOURCES

http://www.arrakis.es/~lluengo/pproteinas.html
http://www.um.es/molecula/prot.htm
http://www.cnice.mecd.es/eos/MaterialesEducativos/mem2002/proteinas/
http://es.wikipedia.org/wiki/Prote%C3%ADna
http://www.arrakis.es/~lluengo/adn.html
http://es.wikipedia.org/wiki/ADNhttp://fai.unne.edu.ar/biologia/macromoleculas/adn.htm
http://ndbserver.rutgers.edu/
http://tigger.uic.edu/~mansoori/Thermodynamics.Educational.Sites_html

ASSESSMENT

Methodology

-Preparation and presentation of reports and assignments.-Resolution of exercises and practical cases-Participation in seminars, tutorials and other activities-Preparation, presentation and defence of an individual assignment.-Completion of assessment tests (final exam)

Marking criteria

Continuous assessment. 40%.
This mark represents an evaluation of the active participation of the student, their answers given to the theoretical-practical cases proposed, the development of laboratory work and, where applicable, the preparation and presentation of reports.
Final exam: 30%
A four-hour final written exam on all of the subject matter, consisting of responses to questions and selected problems.
Preparation and presentation of an assignment. 30%
Each student will prepare a written assignment, which must be presented in public (for 30 minutes) and defended in front of the course lecturers. The subject matter must be chosen from among those proposed by the course lecturers.

PROGRAMMED ACTIVITIES (Course contents and time frame)

Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1	Jose María Leal Villalba	14	4
Unit 2	Saturnino Ibeas Cortés	6.5	2

Unit 3	Begoña García Ruiz	6.5	2
Unit 4	Rafael Alcalde García	7.0	2
Unit 5	Rafael Alcalde García	7.0	2
Unit 6	Francisco Javier Arnáiz García	7.0	2
Unit 7	Francisco Javier Arnáiz García	7.0	2
Unit 8	Saturnino Ibeas Cortés, Begoña García Ruiz	15	4
Exam preparation.		--	30
Completion of final assessment test		5	--
Total	**125**		

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
COMPUTATIONAL CHEMISTRY			5257
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (2/3)

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LECTURER (2)			
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LECTURER (3)			
José Vicente Cuevas Vicario			
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LECTURER (4)			
Miguel Angel Rodríguez Barranco			
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Department	Chemistry	Area	Organic Chemistry
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--	941-299651	miguelangel.rodriguez@dq.unirioja.es	

STUDENT WORKLOAD		HOURS	
		Weekly	Total hours
TAUGHT CLASSES	Attendance at lectures	2	16
	Attendance at practical classes (laboratory or computer room)	2	24
	Attendance at seminars and activities		2
	Attendance at assisted tutorials		4
	Presentation of assignments		2
	Completion of assessment tests		2
PRIVATE STUDY	Group work for theoretical and/or practical classes.	1.5	15
	Study for the preparation of theoretical and/or practical classes.	1	10
	Resolution of exercises and practical cases, preparation of reports and presentations	4	40
	Exam preparation.	1	10
Total hours (Taught Classes)	50	**Total hours (Private Study)**	75
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

-Theoretical models for electronic structure determination.
-Computer implementation of theoretical models: available programmes.
-Practical application: use of Gaussian03 for the study of systems of interest in Chemistry.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

-User-level knowledge of any commonly-used operating system in computing.
-Knowledge of the electronic configurations of atoms and simple molecules.

OBJECTIVES

General

-Search and retrieval, by the student, of paper-based as well as electronic information in the bibliography.
-Encouragement of a critical spirit in the student.
-Improvement of the student's capacity for group work.
-Development of the student's creativity.

Specific

-Comprehension of the different approaches and models currently in use.
-Use of specialized software packages.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

-Use of Gaussian03 by the student.
-Information retrieval from Gaussian03 output files by the student.

-Understanding of the computational section of a research paper.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

-Ability to make a public presentation.
-Ability to prepare easily understandable texts of a scientific nature.

STUDY PROGRAMME

Unit 1. Introduction. General overview of simulation techniques.
Unit 2. Molecular mechanics. Force fields and their parametrization.
Unit 3: Hartree-Fock. The helium atom. Slater determinants. Exchange. Translational symmetry. Configuration interaction (CI, MP).
Unit 4: Periodic systems and plane waves. The Plane-Wave (PW) method. Augmented Plain Waves (APW). Linearised Augmented Plain Waves (LAPW).
Unit 5: Periodic systems and localized bases. Slater bases. Gaussian bases. Contracted bases.
Unit 6: Density Functional Theory (DFT). The Thomas and Fermi (TF) model. Kohn and Sham (KS) equations. Exchange-correlation functionals.
Unit 7: Pseudopotentials Ashcroft. Hamman. Troullier and Martins (TM). Perdew and Fiolhais (PF).
Unit 8: Semiempirical methods. Extended Hückel, CNDO, INDO.
Unit 9. Molecular dynamics. Classic and quantum equations. Integration methods.
Unit 10: Monte Carlo. Integration. Markov chains.

METHODOLOGY

-Lectures
-Topic presentations by students.
-Practical classes using Gaussian03.
-An assignment involving the application of Gaussian03 to a particular system chosen by the student.

BIBLIOGRAPHY

Basic reference works

-*Computational physics*. J.M. Thijssen. Cambridge University Press, 1999.
-*Computer simulation of liquids*. M.P. Allen and D.J. Tildesley. Oxford University Press, 1987.
-*Introduction to Computational Chemistry*. Frank Jensen. John Wieley & Sons, LTD
-*Exploring Chemistry with Electronic Structure Methods* (second edition). James B. Foresman and Æleen Frisch. Gaussian, Inc.

Other bibliographic works to consult

-*Modern quantum chemistry: introduction to advanced electronic structure theory*. A. Szabo and N.S. Ostlund. Dover, 1989.
-*Density-functional theory of atoms and molecules*. R. Parr and W. Yang. Oxford University Press, 1989.
-*Density functional theory: an approach to the quantum many-body problem*. R.M. Dreizler and E.K.U. Gross. Springer Verlag, 1990.
-*Density functional methods in chemistry and materials science*. M. Spingborg (Editor). John Wiley &Sons, 1997.
-*Molecular Modeling of Inorganic Compounds* (Second, completely revised and enlarged

edition). Peter Comba, Trevor W. Hambley. Wiley-VCH, Weinheim, 2001
-*Essentials of Computational Chemistry. Theories and Models*. Christopher J. Cramer. John Wiley & Sons, LTD
-*Molecular Modelling for Beginners*. Alan Hinchliffe. John Wiley & Sons, LTD

INTERNET RESOURCES

-www.gaussian.com
-www.emsl.pnl.gov/forms/basisform.html

ASSESSMENT

Methodology

- The solution of exercises in practical classes.
- Preparation and defense of theoretical assignments.
- An assignment involving the application of Gaussian03 to a particular system chosen by the student.
- A practical exam on Gaussian03.

Marking criteria

- Practical classes to resolve set exercises:	50%
- Presentation of theoretical assignments.	15%
- An assignment involving the application of Gaussian03 to a particular system chosen by the student.	25%
- A practical exam on Gaussian03.	10%

PROGRAMMED ACTIVITIES (Course contents and time frame)

Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1.- Introduction.	Nicolás Cordero	2	2
Unit 2.- Molecular mechanics.	Nicolás Cordero	2	4
Unit 3.- The Hartree-Fock method	Nicolás Cordero Begoña Torres Miguel A. Rodríguez	10	10
Unit 4.- Periodic systems and plane waves.	Begoña Torres	4	7
Unit 5.- Finite systems and localized bases.	José Vicente Cuevas Miguel A. Rodríguez	4	7
Unit 6.- DFT	Begoña Torres Nicolás Cordero	14	14
Unit 7.- Pseudopotentials	Begoña Torres Nicolás Cordero	2	4
Unit 8.- Semiempirical methods.	José Vicente Cuevas Miguel A. Rodríguez	6	7
Unit 9.- Molecular dynamics.	José Vicente Cuevas	2	5
Unit 10.- Monte Carlo.	José Vicente Cuevas	2	5
Exam preparation.	All lecturers	--	10
Completion of final assessment test	All lecturers	2	--
Total		**125**	

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
ORGANIC AND INORGANIC INDUSTRIAL CHEMISTRY			5253
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY.	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Nº credits (T/P)
Second	2	Semi-optional	5 (4/1)

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LECTURER (3)			
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LECTURER (4) IN CHARGE OF THE COURSE			
Felipe Serna Arenas			
Institution/firm	INTERBON S.A.	Centre	Burgos Factory

Department	Chemistry	Area	
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STUDENT WORKLOAD		HOURS	
		Weekly	Total hours
TAUGHT CLASSES	Attendance at lectures	2	30
	Attendance at practical classes (laboratory or computer room)	2	10
	Attendance at seminars and activities	2	10
	Attendance at assisted tutorials	1	5
	Presentation of assignments	1	15
	Completion of assessment tests	1	5
PRIVATE STUDY	Group work for theoretical and/or practical classes.	2	10
	Study for the preparation of theoretical and/or practical classes.	1	15
	Resolution of exercises and practical cases, preparation of reports and presentations	4	20
	Exam preparation.	1	5
Total hours (Taught Classes)	75	**Total hours (Private Study)**	50
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

Technology for obtaining primary products and for their chemical transformation taking account of the economic aspects of organic chemistry at an industrial level. A number of chemical transformations and methods to obtain various products will be studied, as well as environmental aspects, the analysis of primary materials, production processes, products and chemical industry waste products.

PRIOR REQUIREMENTS AND/OR RECOMMENDATIONS

It is recommended that the student have followed a graduate-level course in general chemistry, as well as basic notions of organic, inorganic and physical-chemistry

OBJECTIVES

General

To develop organisational skills in the student, in order to be able to organise, oversee and undertake tasks in the chemical industry; from laboratory-based research or analysis to production in complex industrial installations.
To provide the student with a solid knowledge base and skills to apply to the resolution of qualitative and quantitative skills in industrial development.

Specific

The study of organic and inorganic compounds of technological interest as well as other related-industrial processes.
To understand standard methodological analyses in the chemical industry and to develop the capacity to select the most appropriate to each specific problem.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

Properties of organic, inorganic and organometallic compounds of greatest technological interest. Principal types of chemical reactions and their main associated characteristics.
Capacity to demonstrate knowledge and comprehension of essential facts, concepts, principals and theory related to areas of Chemistry.
Resolution of qualitative and quantitative problems according to a previously developed model.
Ability to recognise and analyse new problems and establish strategies to solve them.
Safe handling of chemical materials.
Plan, design and execute practical research, from the problem-recognition stage up until the assessment and the evaluation of results and discoveries.
Risk assessment in the use of chemical substances and laboratory procedures.
Capacity to generate new ideas.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND SYSTEMATIC).

- Organisational and planning skills
- Problem-solving skills
- Decision-making skills
- Team work
- Critical reasoning
- Autonomous learning
- Quality-driven approach
- Sensitivity towards environmental issues

STUDY PROGRAMME

Unit 1. General aspects of the chemical industry.
The chemical industry in the world, in Europe, in Spain and in Castille and Leon. Principal sectors. Economic importance. Future perspectives for the chemical industry. The chemical industry and the environment.

Unit 2. Inorganic industrial chemistry.
2.1. Water and the chemical industry. Treatments prior to and following its use.
2.2. Industrial gases. Oxygen, nitrogen, hydrogen, and carbon dioxide.
2.3. Metallurgic industry. Metals and alloys. Treatment of ores. Obtaining and purification of metals. Iron and steel. Other metals and alloys. Pirometallurgic processes. Electrochemical processes Environmental aspects.
2.4. The ceramic and glass industry. Silica and silicates. Clay products. Refractory materials. The glass industry. Primary materials. Molding, tempering and finishing. Special glasses.
2.5. The nitrogen derivatives industry. Ammonia, nitric acid and nitrates.
2.6. The phosphorus industry and its derivatives. Phosphoric acid, phosphates and superphophates.
2.7. The sulphur industry and its derivatives. Sulphur, sulphuric acid and sulphates.
2.8. The chloro-alcali industry. Hydroxide and sodium carbonate. Other inorganic processes of industrial interest.

Unit 3. Organic industrial chemistry.
3.1. Production of basic organic compounds. Petroleum and natural gas. Other sources. carbon, fats and oils, carbohydrates.
3.2. The paper industry. Primary materials. Preparation of chemical pastes. Paper manufacturing. Problem of the paper industry. Environmental aspects.
3.3. The pharmaceutical industry. Action mechanisms of medicines. R&D of a

pharmaceutical product.
3.4. The agro-chemical industry. Insecticides. Herbicides. Fungicides. Rodenticides. Fumigants. Nematocides. Ecological agriculture.
3.5. Colorants and pigments. Intermediary products. Azoic colorants. Anthraquinone colorants. Triphenylmethane colorants. Indigoid colorants. Inorganic colorants. Pigments.
3.6. The food industry. Organic chemistry and foodstuffs. Foodstuffs in Castille and Leon. Functional foods. Natural and synthetic additives: conservants, antioxidants, flavour stimulants,…
3.7. Detergents and soaps. Detergent mechanisms. Tensioactives: anionics, cationics, amphoterics and noionics. Additives.
3.8 Civil explosives. Primary and secondary explosives. Synthesis, characterisation and applications

Unit 4. Industrial analysis.
4.1. The analytical laboratory in the chemical industry: structure, functions. Information management systems in the laboratory. Reports Maintenance and reliability of the analytical system.
4.2. Analytical methods used in industry. Continuous and discontinuous analysis. Analysis of raw materials. Chemical analysis of processes. Product analysis. Waste analysis.
4.3. Some methods of special industrial interest. Particle analysis. Analysis of gases. "Lab-on-a-chip" technologies.

METHODOLOGY

The methodology is centred on student learning processes and is adapted to the European Credit Transfer Scheme (ECTS). On this course, the ratio between taught and private study hours is 60/40. Figuring among the taught hours is the lecture, a communication method in which the lecturer is active and the student receptive, which despite all the reservations that have been expressed in this regard, continues to be key to the educational system as, among its other advantages, it is a rapid method to provide information to students who will find the course work more accessible and who would otherwise feel discouraged if they had to approach it merely by reading. It also prepares the student to follow a path towards his or her own research,... However, although lectures are (in our opinion) irreplaceable, they should not be overused for which reason they are coordinated with other less passive activities and techniques that allow for greater student participation. To that end, oral presentations by students in the classroom are proposed, as well as discussion between students. In addition, professional guidance is given in the course of tutorials. Industrial case studies will be presented, frequent visits will be made to regional industries and professionals working in the industry will attend seminars to make presentations on the specific cases of various firms.

BIBLIOGRAPHY

1. Chemical Process Technology, Moulijn at al., Wiley, 2001.
2. Industrial Chemistry, E. Stocchi, Ewllis Horwood, 1990.
3. Introduction a la Quimica industry, A. Vian Ortuño, Reverte, 1994.
4. Industry Inorganic Chemicals: Production and uses, R. Thompson (Ed.), RSC, 1995.
5. Industry Inorganic Chemistry, Buchner et al.VCH, 1989.
6. Productos Químicos Orgánicos Industriales, H. A. Wittcoff, vol 1 and 2. Lumisa, 1994.
7. Química Orgánica Básica y Aplicada. E. Primo Yúfera, vol 1 and 2, Reverte, 1995
8. Industrial Organic Chemistry. K. Weissermel, H.-J. Arpe, Wiley-VCH, 1997.
9. Chemistry and Technology of Explosives". Volumes 1 to 4. T. Urbanski, Pergamon Press, 1990.
10. Curso de Tecnología de Explosivos, J. A. Sanchidrián and E. Muñiz, Servicio de Publicaciones de la Fundación Gómez-Pardo. Escuela Técnica Superior de Ingenieros de Minas, Universidad Politécnica de Madrid, 2000.

ASSESSMENT
Methodology
– Preparation and presentation of reports and assignments. – Resolution of exercises and practical cases – Participation in seminars, tutorials and other activities – Completion of assessment tests
Marking criteria
– Proposed marking criteria: – Participation in classes, seminars and complementary activities: 30 % – Preparation and presentation of assignments 40 % – Final Exam 30 %.

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught Classes	Private study
Unit 1.-	Javier Arnáiz García	1 Lect.	---
Unit 2.-	Javier Arnáiz García	12 (Lects.)5 (P.)2 (T.)6 (P.A.)	18
Unit 3.-	María García Valverde	11 (Lect.)5 (P.)2 (T.)6 (P.A.)	18
Unit 4.-	Jesús López Palacios	6 (Lects.)1 (T.)10 (Other)3 (P.A)	9
Exam preparation.			5
Completion of final assessment test		5	--
Total	**125**		

Lects. Lectures P. Practicals: T. Tutorials Other activities: P.A. Presentation of Assignments

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
GREEN CHEMISTRY AND SUSTAINABLE DEVELOPMENT			5252
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY.	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Nº credits (T/P)
Second	2	Semi-optional	5 (3/2)

LECTURER (1) IN CHARGE OF THE COURSE			
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STUDENT WORKLOAD	HOURS	
	Weekly	Total hours

TAUGHT CLASSES	Attendance at lectures	2	30
	Attendance at practical classes (laboratory or computer room)	1	15
	Attendance at seminars and activities	10/15	10
	Attendance at assisted tutorials	5/15	5
	Presentation of assignments	10/15	10
	Completion of assessment tests	5/15	5
PRIVATE STUDY	Group work for theoretical and/or practical classes.	10/15	10
	Study for the preparation of theoretical and/or practical classes.	1	15
	Resolution of exercises and practical cases, preparation of reports and presentations	20/15	20
	Exam preparation.	5/15	5

Total hours (Taught)	75	**Total hours (Private Study)**	50
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

- Environmental contamination.
- Process optimization.
- Atomic economy.
- Alternative reactives.
- Alternative technologies.
- Catalysis.
- Ionic liquids.
- Supercritical fluids.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

It is recommended that the student have studied chemistry for at least two semesters.

OBJECTIVES

General

- To develop the capacity of the student to value the importance of chemistry in industrial, economic, environmental and social contexts.
- To develop the capacity of the student to organise, oversee and undertake tasks in the chemical industry, ranging from laboratory research or analysis to production in complex industrial plants, paying special attention to the minimization of residues.
- To provide students with a solid knowledge base and abilities which they can apply to the resolution of environmental problems related to chemical processes.

- Specific

- To generate in students the capacity to value the importance of a "greener" chemistry within the context of sustainable development.
- To provide students with a knowledge series related to the use of alternative technologies in chemical processes and the minimization of residues.
- The preparation of especially appropriate techniques to resolve environmental problems in the modern chemical industry.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

- Safe handling of chemical materials.
- Principal aspects of chemical terminology, nomenclature, agreements and units.
- Metrology of chemical processes including quality assurance management.
- Principal types of chemical reactions and their main associated characteristics.
- Ability to recognise and analyse new problems and establish strategies to solve them.
- Risk-assessment skills in the use of chemical substances and laboratory procedures.
- Ability to evaluate, interpret and summarise chemistry-related data and information.
- Ability to carry forward standard laboratory procedures involved in synthetic work in relation to organic and inorganic systems.
- Ability to demonstrate knowledge and comprehension of essential facts, concepts, principals and theory related to areas of Chemistry.
- Ability to plan, design and execute practical research, from the problem-recognition stage up until the assessment and the evaluation of results and discoveries.
- Ability to interpret information taken from laboratory observations and measurements in terms of its meaning and the theories that support it.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Organisational and planning skills.
- Problem-solving skills.
- Analytical and summary skills.
- Decision-taking skills.
- Team work.
- Critical and self-critical capacity.
- Autonomous learning.
- Motivated by quality.
- Sensitivity towards environmental issues.
- Ability to recognize and assess chemical processes in daily life.
- Capacity to generate new ideas.
- Capacity to interrelate chemistry and other disciplines.

STUDY PROGRAMME

Unit 1: "**The principles and concepts of Green Chemistry**. Chemistry in the context of sustainable development. Actual state and future perspectives. The twelve principles. Atomic economy. Toxicity and its measurement"
Unit 2: "**Residues and subproducts in the chemistry industry**. Sources of residues. Techniques for its minimization. *In situ* treatment of residues. Design of degradable products"
Unit 3: "**Measuring the environmental impact**. Evaluation of a product lifecycle. ISO 14001. Ecolabels. Legislation. The IPPC directive"
*Unit 4: "**Catalysis and Green Chemistry**.* Introduction to catalysis. Homogeneous and heterogeneous catalyzers. Phase-transfer catalysis. Biocatalysis"
Unit 5: "**Alternative solvents**. Volatile organic compounds Supercritical fluids. Alternatives in extraction and chromatography. Liquid ionics. types, properties and applications"
Unit 6: "**Renewable raw materials**. Biomass and energy. Chemical products based on renewable sources"
Unit 7: "**Green technology and sources of alternative energy**. Photochemical reactions.

Microwaves. Sonochemistry. Electrochemistry"
Unit 8: "The future of Green Chemistry. Alternative designs of processes. Examples of industrial applications. Legislation."

METHODOLOGY

- Lectures using a variety of techniques, especially slides and Power
- Point presentations.
- Laboratory practicals consisting in experiments that demonstrate the principles of Green Chemistry.
- Seminars dealing with the resolution of exercises and problems related to the most significant points set out in the lectures.
- Student assignments on different topics related to Green Chemistry to be presented in public.
- Tutorials to review and discuss the material and themes presented in the course of the lectures.

BIBLIOGRAPHY

Basic reference works

"Green Chemistry: Theory & Practice", P. T. Anastas & J. C. Warner; Oxford University Press, Oxford, 1998.
"Green Chemistry: Frontiers in Benign Chemical Synthesis and Processes", P. T. Anastas et al. (Eds.); Oxford University Press, Oxford, 1998.
"Green Chemical Synthesis and Processes", P. T .Anastas, L G. Heine & T. C. Williamson (Eds.); ACS Symp. Series 767, ACS 2000.
"Green Chemistry: Challenging Perspectives", P. Tundo & P. T. Anastas (Eds.); Oxford University Press, Oxford 2000.
"Real World Cases in Green Chemistry", Michael C. Cann and Marc E. Connelly; ACS, Washington, 2000.
"Introduction to Green Chemistry. Instructional Activities for Introductory Chemistry", M. A. Ryan & M. Tinnesand (Eds.); ACS, Washington, 2002.
"Green Chemistry. An Introductory Text", M. Lancaster, RSC, Cambridge, 2002.
"Greener Approaches to Undergraduate Chemistry Experiments", Mary Kirchhoff and Mary Ann Ryan, ACS, Washington, 2002 (translated into Spanish as 'Química Verde: Experimentos de Laboratorio para un Curso Universitario de Química')" New Trends in Green Chemistry", V. K. Ahluwalia, M. Kidway, Kluwer, 2004.

Other bibliographic works to consult

Books:
"Fundamentals of Supercritical Fluids", Tony Clifford; Oxford Press, NY, 1999.
"Handbook of Green Chemistry and Technology", J. H. Clark & D. Macquarry; Blackwell, Oxford, 2002.
"Supercritical Fluid Extraction" (2nd Edition),McHugh Mark and Krukonis Val J.; Elsevier, 1994.
"Supercritical Fluid Cleaning. Fundamentals, Technology and Applications", John McHardy and Samuel P. Sawan Noye Publications; Westwood, New Jersey, 1998.
"Green Plastics", E. S. Stevens; Princeton University Press, Princeton, 2002.
"Organic Reactions in Aqueous Media", C.-J. Li, T.-K. Chan; John Wiley & Sons, New York, 1997.
"Green Organic Chemistry: Strategies, Tools and Laboratory Experiments" K. M. Doxsee and J. E. Hutchison; Brooks / Cole, 2004.
Articles:
"News from Online: Green Chemistry" E. S. Uffelman, *J. Chem. Ed.* 2004, *81*, 172.

"Green Chemistry, The Sonochemical Approach" P. Cintas and J. L. Luche, *Green Chemistry* 1999, *1*, 115.
"Microwave Assisted Organic Synthesis – A Review" P. Lindstrom, J. Tierney, B. Wathey and J. Westerman, *Tetrahedron* 2001, *57*, 9222.
"Biotechnology for the Production of Commodity Chemicals from Biomass" H. Danner and R. Braun, *Chem. Soc. Rev.* 1999, *28*, 395.
"Solvent-Free Organic Synthesis" K. Tanaka and F. Toda, *Chem. Rev.* 2000, *100*, 1025.
"Chlorine: the only green element – towards a wider acceptance of its role in natural cycles" N. Winterton, *Green Ghemistry* 2000, *2*, 173.
Journals:
Green Chemistry, RSC, 1999.

INTERNET RESOURCES

http://www.epa.gov/
http://www.esig.org
http://www.chemsoc.org/networks/gcn/
http://www.iac.org.uk
http://physchem.ox.ac.uk/MSDS/
http://www.cdc.gov/niosh/ipcs/icstart.html
http://ull.chemistry.uakron.edu/erd/
http://toxnet.nlm.nih.gov/
http://solvdb.ncms.org/SOLV01.htm

ASSESSMENT

Methodology

-Preparation and presentation of reports and assignments.
-Resolution of exercises and practical cases
-Participation in seminars, tutorials and other activities
-Completion of assessment tests (final exam)

Marking criteria

- Preparation and presentation of reports and assignments.
- Resolution of exercises and practical cases (15 %)
- Participation in seminars, tutorials and other activities (15 %)
- Completion of assessment tests: final exam (40 %).

In all cases, the student will be able to obtain a pass in the subject by passing the final exam which will include questions relating to the different activities undertaken throughout the course of study.

PROGRAMMED ACTIVITIES (Course contents and time frame)

Contents	Lecturer/s in charge	Hours	
		Taught Classes	Private study
Unit 1.	Francisco J. Arnáiz	9	6
Unit 2.	Francisco J. Arnáiz	9	6
Unit 3.	Francisco J. Arnáiz	9	6
Unit 4.	Roberto Sanz Diez	12	8
Unit 5.	Rafael Alcalde	10	6
Unit 6.	Roberto Sanz	6	4

Unit 7.	Roberto Sanz	10	6
Unit 8.	Rafael Alcalde	5	3
Exam preparation.		--	5
Completion of final assessment test		5	--
Total	**125**		

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
Seminars • **Public funding for Research & Development & innovation (R&D&i).** • **Safety and hygiene at work.** • **Management.** • **Advanced chemistry in firms and at public research centres.** • **Chemistry and energy.**			5258
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY.	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1 & 2	Semi-optional	5 (5/0)

LECTURER (1) IN CHARGE OF THE COURSE			
Dr. Felipe Serna Arenas (Head of R+D+i at Interbon S.A.)			
Institution/firm	Interbon S.A. / University of Burgos	Centre	Burgos Factory/Faculty of Sciences
Department		Area	
Office	Tel. num. (Ext.)	Email	
1B11	947 25 80 85	fserna@ubu.es	

STUDENT WORKLOAD		HOURS	
		Weekly	Total hours
TAUGHT CLASSES	Attendance at lectures	--	--
	Attendance at practical classes (laboratory or computer room)	--	--
	Attendance at seminars and activities	2	30
	Attendance at assisted tutorials	1	15
	Presentation of assignments		
	Completion of assessment tests	1	15
PRIVATE STUDY	Group work for theoretical and/or practical classes.	--	--
	Study for the preparation of theoretical and/or practical classes.	1h every 3 weeks	5
	Resolution of exercises and practical cases, preparation of reports and presentations	4	60

	Exam preparation.		--	--
Total hours (Taught Classes)	60	**Total hours (Private Study)**	65	
Total hours (Taught Classes and Private Study)	125			

COURSE CONTENTS (DESCRIPTORS)

Seminars on:

- Public funding for R&D&i.
- Safety and hygiene at work.
- Management.
- Advanced chemistry in firms and at public research centres.
- Chemistry and energy.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

No prerequisites or prior recommendations.

OBJECTIVES

General

To bring the student closer to aspects of chemistry that are not dealt with specifically in subjects on the Master's Degree. This implies offering the student a broader and more of a multidisciplinary view of chemistry.

Specific

To offer information to the student on: public funding for R&D&i, safety and hygiene in the workplace, management, advanced chemistry in the firm and at public research centres and chemistry and energy.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

- To learn by example to deliver conferences on various aspects of chemistry-related disciplines.
- The application of academically-acquired theoretical and practical knowledge on chemistry in productive discussions with fellow students.
- Assessment of the need to acquire new knowledge in the light of the topics and applications covered by speakers. Autonomous learning skills to acquire such knowledge.
- Originality and creativity in the use of chemical knowledge when proposing questions and approaches that could hypothetically resolve the problems that might arise in a typical firm or in the conference speaker's own firm.
- Ability to adapt theoretical knowledge for use in a short, concise report that also includes a personal assessment based on scientific foundations on the topic and the way of approaching it at a conference, seminar, or workshop.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Ability to interrelate different disciplines and to prepare short summaries for events such as conferences and other relatively prolonged activities.
- Oral and written communication skills in Spanish, with special emphasis on the delivery of questions in public and the maintenance of productive scientific discussion.

- Ability to search for and retrieve information at all levels, a capacity to summarise such information and to prepare and produce reports.
- Aptitude for autonomous learning and self-study.
- Skills related to computer tools and information technology.
- Interpersonal skills, appropriate for interpersonal relations and for integration in work groups (leadership capacity and decision-making skills).

STUDY PROGRAMME

Conferences on various aspects of chemistry, specifically on:

- Public funding for R&D&i.
- Safety and hygiene at work.
- Management.
- Advanced chemistry in firms and at public research centres.
- Chemistry and energy.

METHODOLOGY

Talks, seminars, roundtables and visits to firms and public research centres.

ASSESSMENT

Methodology

The student must be present for the number of hours at seminars, conferences and workshops as indicated in the programme. An attendance register will be taken at conferences. Furthermore, a report of about 500 words on each activity will be prepared, and a personal assessment of around 100 words will be added at the end of the report. This information will be handed in at the end of the course to the Lecturer/s in charge of the subject, who will assess it.

Marking criteria

Attendance at conferences and the completion of the reports will give students a minimum mark of 5 out of 10. The Lecturer/s in charge of the subject will assess the reports that are handed in by students and give them a mark of between 5 and 10.

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
ADVANCED TECHNIQUES I: X-RAY TECHNIQUES AND MASS SPECTROMETRY			5259
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY.	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (3T/2P)

LECTURER (1) IN CHARGE OF THE COURSE			
Martín Martínez Ripoll			
Institution/firm	Consejo Superior de Investigaciones Científicas (CSIC)	Centre	
Department	Chemistry	Area	Physical Chemistry
Office	Tel. num. (Ext.)	Email	
		xmartin@iqfr.csic.es	

LECTURER (2)			
Mariano Laguna Castrillo			
Institution/firm	CSIC	Centre	Instituto de Ciencia de Materiales de Aragón (ICMA)
Department	Organic Chemistry	Area	Organic Chemistry
Office	Tel. num. (Ext.)	Email	
		mlaguna@posta.unizar.es	

LECTURER (3)			
José Luis Peña Albillos			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Organic Chemistry
Office	Tel. num. (Ext.)	Email	
		jluis@ubu.es	

STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures		30
	Attendance at practical classes (laboratory or computer room)		18
	Attendance at seminars and activities		9
	Attendance at assisted tutorials		9
	Presentation of assignments		3
	Completion of assessment tests		6
PRIVATE STUDY	Group work for theoretical and/or practical classes.		10
	Study for the preparation of theoretical and/or practical classes.		15
	Resolution of exercises and practical cases, preparation of reports and presentations		15
	Exam preparation.		10
Total hours (Taught Classes)	75	**Total hours (Private Study)**	50
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

This module covers the basic aspects of the methods, their scope, different methodologies, innovations, the interpretation of mass spectres and different diffractograms and applications in inorganic and organic chemistry, the environment, biochemistry, toxicology, petrochemistry, medicine, food chemistry and natural products of mass spectrometry and X-ray diffraction analysis.

PRERREQUISITES AND/OR PRIOR RECOMMENDATIONS

Directed at postgraduate students, particularly at chemists, pharmaceutical chemists, analytical chemists, technicians, petrochemical, biochemical and chemical engineers, forensic chemists and professionals in the areas of production, environmental control and other areas with a basic knowledge of chemistry and instrumental analytical techniques, in general.

OBJECTIVES

General

- To widen the students' basic knowledge of mass spectrometry as well as to introduce them to the different spectrometric X-ray techniques, commonly used in chemistry, and to provide them with an overview of the current state of these techniques and on their most recent advances.
- To understand the potential of the EM and X-rays as strategies in the synthesis and characterisation of inorganic compounds, as well as the possibilities in organic chemistry and related fields such as those of synthetic polymers, biomolecules and materials in general and, in other fields, such as tools for chemical analysis used in production processes and other global systems – methods detailed in legislation for forensic chemistry, pharmacology, industrial waste, doping, etc. —.

Specific

- To gain familiarity with the different sources, analysers and detectors used in mass spectrometry, as well as the most appropriate combination of techniques for the characterisation and identification of different types of compounds.

- To select the most appropriate MS parameters for the resolution of concrete problems.
- To interpret the mass spectres that are recorded correctly. To describe the most common experiments with special emphasis on the information contributed by each one and its possible applications.
- To recognise the information contributed by the spectroscopic technique that is used on the structure, the reaction mechanisms and/or the inter- and intramolecular processes presented by the synthesised compounds.
- To learn to design the most appropriate strategy for the characterisation of a compound using this spectroscopic technique.
- To recognise the relation between the results derived from the characterisation of a compound and the synthesis of a new compound.
- To acquire experience in the design, following the analytical stage, of different synthetic possibilities.
- To recognise the importance of the structural crystallography and the way it complements other spectroscopic techniques.
- To distinguish between and assess the advantages and applicability of powder and monocrystal diffractometry, as well as X-ray fluorescence in crystalline and amorphous solids.
- To gain familiarity with techniques to resolve Chemical Structure using monocrystalline and powder diffractometry: resolution strategies.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

- Knowledge of the different sources, analysers and detectors used in mass spectrometry, as well as the most appropriate combination of techniques for the characterisation and identification of different types of compounds.
- Ability to select the most appropriate MS parameters for the resolution of concrete problems. Ability to arrive at a correct interpretation of the mass spectres that are recorded. Ability to describe the most common experiments with special emphasis on the information that each one of them brings and their possible applications.
- Familiarity with the information contributed by the spectroscopic technique that is used on the structure, reaction mechanisms and/or inter- and intramolecular processes presented by the synthesised compounds.
- Ability to design the most appropriate strategy for the characterisation of a material using this spectroscopic technique. Experience at recognising the relation between the results derived from the characterisation of a compound and the synthesis of a new compound.
- Acquisition of experience in the design, following the analytical stage, of different synthetic possibilities.
- Ability to recognise the importance of structural crystallography and the way it complements other spectroscopic techniques.
- Ability to distinguish between and assess the advantages and applicability of both powder and monocrystalline diffractometry, as well as X-ray fluorescence in crystalline and amorphous solids.
- Familiarity with techniques to resolve Chemical Structure using monocrystalline and powder diffractometry: resolution strategies.
- Strengthen the ability of the student to identify which specific experiment could be useful at a given moment to obtain precise information.
- Develop the knowledge and abilities of the student that are needed to modify the experiment, or design a new one, based on the results obtained with the aim of broadening the available information in relation to a compound or a particular experiment.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND SYSTEMATIC).
– To increase the capacity for group work and to communicate both within and outside the classroom with the rest of the group in an interdisciplinary setting. – Introduce communication – in different ways - on the results of personal work into learning practices. – To be familiar with and to use different bibliographic sources as interdisciplinary working tools needed to develop work of a different type: theoretical, experimental, and applied research. – Acquire the skills neeeded to prepare a written report. – Compare and discriminate between the *theoretical,* the *experimental* and the *real* in the context of learning. – Acquire the capacity to approach a new topic of work and develop it. – Accept the importance of active participation and personal work in the final results relating to acquired knowledge as well as to any improvement in the overall mark. – Arrive at an acceptable interpretation of the results or experimental evidence in relation to the theoretical basis upon which they are founded.

STUDY PROGRAMME	
Unit 1.	Introduction to MS. Ionization methods. Sources: electronic impact, chemical ionization, FAB, LSIMS, Electrospry, etc.
Unit 2.	Analyzers: magnetic and electromagnetic, quadrupoles, time-of-flight, cyclotrons as well as other combined techniques.
Unit 3.	Ion detection and data treatment systems.
Unit 4.	Different interfaces: chromatography-mass spectrometry, electrophoresis-mass spectrometry, tandem MS/MS.
Unit 5.	Information for the structural elucidation of inorganic/organic compounds: base peaks, parent peaks, fragmentations, aggregations, isotopical distributions.
Unit 6.	Spectral interpretation.
Unit 7.	Equipment: Gas Masses in the Area of Organic Chemistry and SCAI scanner High Resolution Masses (Uni. Burgos R&D&i)
Unit 8.	The most frequent and/or recent mass spectrometry applications.
Unit 9.	Introduction and objectives of crystallography. General concepts Networks, planes, indices, symmetry. Point and space groups.
Unit 10.	Dispersion phenomena. Physical and geometric aspects of diffraction.
Unit 11.	X-ray generation. Conventional tubes, rotating anodes and synchroton rings.
Unit 12.	The structural factor. Diffraction symmetry. Systematic extinctions.
Unit 13.	Goniometers and detectors. Intensity measurements. Analysis of the spectre
Unit 14.	Resolution of tridimensional structures. The phase problem. Phase assignment methods.
Unit 15.	Structural determination using vectorial and direct methods.
Unit 16.	The use of structural databases.
Unit 17:	The extension of crystallography to biological macromolecules. Structural databases.

METHODOLOGY

The course has a theoretical and a practical component, both of which are closely interconnected. The theoretical sessions will take place with a high degree of student participation. In addition to analysing theoretical concepts introduced by the lecturer, students will simultaneously discuss the experimental spectroscopic data that illustrate them. The course ends with a series of practical sessions, to be carried out on the equipment with the help of the lecturer, in which some of the eminently practical concepts are demonstrated on an experimental basis that students will encounter when using these techniques. Some of the sessions will include individual problem-solving activates on specific aspects of the technique and well as aspects set within its combined application in the fields of synthesis and characterisation.

Lectures will be successively interspersed between taught classes in the laboratory — applications, sample preparations, recording spectra and readings on the diffractometer, etc. — as well as in seminars that will be held to resolve a number of practical proposals in some cases as well as to defend the assignments set as projects. The tutorials will respond to the individual expectations of the students as well as serving to clarify concepts and to provide students with a series of work patterns so that they may express their problems and try to solve them in the presence of the lecturer.

In addition, an on-line working method will be set up with each one of the students with a view to conducting continuous assessment of their learning achievements as this means of communication allows on-line tutoring at times that are more convenient for both student and lecturer.

The system of continuous evaluation consists of the complete set of activities, which includes the written tests from the start up until the completion of the assignment and the student's replies.

BIBLIOGRAPHY

Basic reference works

- *Interpretation of Mass Spectra*. F.W. McLafferty and F. Turecek, University Science Books, Mill Valley, CA, 4th, 1993
- *Mass Spectrometry. Principles and Applications*. E. de Hoffmann, J. Charette and V. Stroobant (2nd.), Wiley, 2001
- *Experimental Mass Spectrometry*, D.H. Russel, Plenum Press, New York, 1994
- *La espectrometría de masas en imágenes*, L. Esteban (Ed.), ACR, New York, 1993.
- *Tandem Mass Spectrometry*, F.W. McLafferty, Viley, 1983.
- *Inorganic Mass Spectrometry*, F. Adams, R. Gijbels and R. van Grieken, John Wiley, New YorK, 1988.
- *Applications of Mass Spectrometry to Organic Stereochemistry*. Edited by Janet S. Splitter and Frantisek Turecek, Wiley-VCH, New York, 1993.
- *Mass Spectrometry of Polymers*, Edited by G. Montaudo and R. Lattimer, CRC Press, New York, 2001.
- *Techniques for the Study of ion-molecule Reactions*, J.M. Farrar and W.H. Saunders, Wiley, New York, 1988.
- *Analytical Pyrolysis of Natural Organic Polymes*, S.C. Moldoveanu, ElsevierNew York, 1998.
- *Spectroscopy Europe*. IMPublications, Wiley (Periodically published at www.spectroscopyeurope.com)
- *X-Ray Crystallography*, M. M. Woolfson, Cambridge University Press, 1997.
- *X-Ray Structure Determination. a practical guide*, G. H. Stout, L. H. Jensen, Wiley,

BIBLIOGRAPHY

Basic reference works

1989.

- *Crystal Structure Determination,* William Clegg, Ed. Oxford University Press, Oxford, 1998.
- *The Basics of Crystallography and Diffraction,* Christopher Hammond**,** Oxford University Press, Oxford, 1997. (IUCr Texts on Crystallography 3)
- *Fundamentals of Crystallography* C. Giacovazzo et al, Ed. Oxford Science Publications (IUCr), Oxford, 1992 (1st edition). 2002 (2nd edition).
- *Crystal Structure Analysis for Chemists and Biologists,* Jenny P. Glusker, Mitchell Lewis and Miriam Rossi, Ed.VCH, New York, 1994.
- L.V. Azaroff. *Elements of X-ray Crystallograph.* McGraw-Hill Book 1968
- G. Harbour, C.A. Taylor, T.R. Welberry. *Atlas of Optical Transforms.* Bell, London
- J. Pickworth Glusker, K.N. Trueblood. *Crystal Structure Analysis: A primer.* Oxford University Press, 1985
- G.H. Stout, L.H. Jensen. *X-ray structure determination: a practical guide.* The Macmillan Company, 1989
- Hermoso, J.A. and Martínez-Ripoll, M. *Estructura de proteínas por Cristalografía de rayos X.* In "Estructura de proteínas" (Gómez-Moreno, C. and Sancho Sanz, J., coord.), Ariel Ciencia. Madrid, 2003

Other bibliographic works to consult

- *Spectroscopy Europe*. IMPublications, Wiley (Also, periodically published at www.spectroscopyeurope.com)
- American Society for Mass Spectrometry
- http://www.asms.org/
- SpectroscopyNow.com
- http://www.spectroscopynow.com/coi/cda/home.cda?chId=0
- The crystallography of X-rays
- http://www.xtal.iqfr.csic.es/Cristalografia/index2.html

– INTERNET RESOURCES

- American Society for Mass Spectrometry
  http://www.asms.org/

- SpectroscopyNow.com
- http://www.spectroscopynow.com/coi/cda/home.cda?chId=0

- The crystallography of X-rays
  http://www.xtal.iqfr.csic.es/Cristalografia/index2.html

- On-line teaching-learning platform of the UBU (e-campus)
  https://ubunet.ubu.es/co/pag/index.htm

- The student's electronic file through the UBUNET (Virtual Campus, personal/academic link that includes forums for students enrolled via a UBU email address)
  https://ubunet.ubu.es/co/pag/index.htm

- Access to the library and its services through the Off-Campus

http://www.ubu.es/biblioteca/off-campus/index.htm

ASSESSMENT
Methodology
A personalised follow up of each student will take place, monitoring progress throughout the course (Continuous assessment), the level at which concepts are assimilated, the student's capacity to put them into practice in an effective manner, the level of participation in the different sessions and the student's overall progress and degree of maturity. This assessment takes place both in the theoretical component and in the set theoretical-practical case studies, as well as in the final practical component at the end of the course. The student must have full knowledge of and select the most appropriate of the different experiments available for each particular case, with a view to obtaining specific information and, subsequently, interpreting the results — the responses contributed in each problem will be assessed in at least in 20% of the programme of taught classes that are not lectures. To that end, the answers to exercises and practical cases are assessed through the corresponding reports handed in and defended by students in taught classes - seminars, tutorials, laboratory practicals – as well as the results of their off-campus work using the on-line platform. At the end of the course, in addition, the student will have to solve a *problem* that includes the application of all the knowledge considered as global strategies in the synthesis and characterization of a problem compound proposed by the lecturer – a formal written exam in a classroom setting.
Marking criteria
The answers given to exercises and practical cases (including Assignments or Projects and their defence) assessed on the basis of the corresponding reports handed in and defended by students in taught classes - seminars, tutorials, laboratory practicals — [40% of the total mark], as well as the results of their off-campus work using the on-line platform [30% of the total]. The correct resolution of a set *problem* at the end of the course that includes aspects that have been considered on the course ranging from mass spectrometry to X-ray spectroscopy [30% of the total].

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 1. Introduction to MS. Ionization methods. Sources: electronic impact, chemical ionization, FAB, LSIMS, Electrospry, etc.	Prof. Mariano Laguna Castrillo	**6**	**6**
Unit 2. Analyzers: magnetic and electromagnetic, quadrupolars, time-in-flight, cyclotrons and other combined techniques.	Prof. Mariano Laguna Castrillo	**4**	**3**
Unit 3. Ion detection and data treatment systems.	Prof. Mariano Laguna Castrillo	**3**	**2**
Unit 4. Different interfaces: chromatography-mass spectrometry, electrophoresis-mass spectrometry, tandem MS/MS.	Prof. Mariano Laguna Castrillo and Dr. José Luis Peña Albillos	**4**	**3**
Unit 5. Information for the structural elucidation of inorganic/organic compounds: base peaks, parent peaks, fragmentations, aggregations, isotopical distributions.	Prof. Mariano Laguna Castrillo and Dr. José Luis Peña Albillos	**8**	**7**
Unit 6. Spectral interpretation.	Prof. Mariano Laguna Castrillo and Dr. José Luis Peña Albillos	**6**	**5**
Unit 7. Equipment: Gas Masses in the Area of Organic Chemistry and SCAI scanner High Resolution Masses (Uni. Burgos R&D&i)	Dr. José Luis Peña Albillos	**7**	**4**
Unit 8. The most frequent and/or recent mass spectrometry applications. Unit.	Prof. Mariano Laguna Castrillo and Dr. José Luis Peña Albillos	**6**	**5**
Unit 9. Introduction and objectives of crystallography. General concepts Networks, planes, indices, symmetry. Point and space groups.	Prof. Martín Martínez Ripoll	**2**	**2**
Unit 10. Dispersion phenomena. Physical and geometric aspects of diffraction.	Prof. Martín Martínez Ripoll	**2**	**1**
Unit 11. X-ray generation. Conventional tubes, rotating anodes and synchroton rings.	Prof. Martín Martínez Ripoll	**2**	**1**
Unit 12. The structural factor. Diffraction symmetry. Systematic extinctions.	Prof. Martín Martínez Ripoll	**3**	**1**
Unit 13. Goniometers and detectors. Intensity measurements. Spectrum analysis.	Prof. Martín Martínez Ripoll	**3**	**1**

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught classes	Private study
Unit 14. Resolution of tridimensional structures. The phase problem. Phase assignment methods.	Prof. Martín Martínez Ripoll	**3**	**3**
Unit 15. Structural determination using vectorial and direct methods.	Prof. Martín Martínez Ripoll	**3**	**2**
Unit 16. The use of structural databases.	Prof. Martín Martínez Ripoll	**2**	**2**
Unit 17: The extension of crystallography to biological macromolecules. Structural databases.	Prof. Martín Martínez Ripoll	**2**	**2**
Group work for theoretical and/or practical classes.		**—**	**10***
Study for the preparation of theoretical and/or practical classes.		**—**	**15***
Resolution of exercises and practical cases, preparation of reports and presentations		**—**	**15***
Exam preparation.		**—**	**10***
Presentation of assignments	Prof. Martín Martínez Ripoll Mariano Laguna Castrillo and Dr. José Luis Peña Albillos	**3**	
Completion of final assessment test	Prof. Martín Martínez Ripoll Mariano Laguna Castrillo and Dr. José Luis Peña Albillos	**6**	**--**
Total	**125**		

***The total of 50 hours of private study corresponds to the estimates for each unit that only involve private study.**

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
ADVANCED TECHNIQUES II: MULTINUCLEAR MAGNETIC RESONANCE, ELECTRONIC PARAMAGNETIC RESONANCE AND MOLECULAR MAGNETISM			5260
Title	Centre		
MASTER's IN ADVANCED CHEMISTRY.	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	2	Semi-optional	5 (3/2)

LECTURER (1) IN CHARGE OF THE COURSE			
Javier García Tojal			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Inorganic Chemistry
Office	Tel. num. (Ext.)	Email	
QI-22 (294)	947 258035	qipgatoj@ubu.es	

LECTURER (2)			
Rafael Aguado Bernal			
Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Chemistry	Area	Inorganic Chemistry
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QI-13 (282)	947 258035	raguado@ubu.es	

LECTURER (3)			
Luis Mª Lezama Diago			
Institution/firm	Universidad del Pais Vasco	Centre	Faculty of Science and Technology
Department	Inorganic Chemistry	Area	Inorganic Chemistry
Office	Tel. num. (Ext.)	Email	
	94 6012703	qipledil@lg.ehu.es	

STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	3	45
	Attendance at practical classes (laboratory or computer room)	0.7	10
	Attendance at seminars and activities	0.7	10
	Attendance at assisted tutorials	0.7	10
	Presentation of assignments	0.3	5
	Completion of assessment tests	0.3	5
PRIVATE STUDY	Group work for theoretical and/or practical classes.	0.3	5
	Study for the preparation of theoretical and/or practical classes.	1.4	20
	Resolution of exercises and practical cases, preparation of reports and presentations	0.7	10
	Exam preparation.	0.3	5

Total hours (Taught Classes)	85	**Total hours (Private Study)**	40
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

- Multinuclear-magnetic-resonance spectroscopy (MRS).
- Molecular magnetism
- Electron-paramagnetic-resonance spectroscopy (EPR).

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

It is recommended that the student possess knowledge of physics and chemistry at graduate level.

OBJECTIVES

General

- To understand the fundamentals, concepts, limits and essential ideas of the techniques.
- To know how to design systems and appropriate experiments so that students may apply what they learn to their area of research.
- To learn to interpret the results obtained and, if necessary, to redesign new systems and/or experiments that transmit more information.

- Specific

- To gain familiarity with the different techniques available to the student and the relevant experiments to conduct, knowing the information that each one of them may provide. Likewise, to understand the factors that affect the magnetic properties of the systems.
- Acquire the knowledge to select which experiment or set of experiments is the most appropriate to obtain the desired information, as well as to design systems that present particular properties.
- Finally, to interpret and to analyse the results obtained, and on that basis to design new experiments or systems to obtain additional information or undertake the necessary modifications.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

The course will enable the student to:

- Gain sufficient knowledge and ability to correctly use the resonance and magnetism techniques that are under study, being aware of their possibilities and limitations.
- Gain skills needed to acquire experimental abilities that lead to the assimilation of other more complex ones.
- Be able to prepare a technical report that is comprehensible to anybody that has received a scientific training but is not an expert in the subject.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Problem-solving skills relating to qualitative and quantitative information.
- Skills involving the application of theoretical knowledge in practical work.
- Oral and written communication skills in the student's first language
- Ability to search for and retrieve information, whether through primary or secondary sources, including information obtained through on-line communication and through access to data banks.
- Abilities to summarise to prepare and present reports.
- Abilities and skills in practical aspects, manual abilities at undertaking tasks.
- Study skills and autonomous learning, necessary for continuous training and professional development
- Skills related to computer tools and information technology (such as, word processing skills, spread sheets, databases, internet communications, etc.)
- Interpersonal skills, appropriate for relating to other people and for integration in work groups.
- Ability to work in a group.
- Decision-making skills.
- Ability to perform numerical calculations, including aspects such as evaluation of the magnitude and its orders, the correct use of the measurement unit, error analysis, statistical estimates, etc.
- Ability to integrate quality as one of the most important variables to consider in day-to-day work.
- Deductive reasoning skills and the ability to exploit creative thinking, through their introduction into research.
- Ability to recognise the need to show respect for the life and wellbeing of people and respect for the environment as primordial patterns of professional conduct.

STUDY PROGRAMME

Unit 1. Multinuclear magnetic resonance spectroscopy (MRS).

Theoretical:

Introduction to MRS. MRS Equipment. Relaxation phenomena. Chemical screening and displacement. Coupling and coupling constants. Spin systems: ^{13}C MRS : pulse techniques, NOE (Nuclear Overhauser Effect). The application of MRS to organometallic fields. MRS dynamics. Modern mono and bidimensional experiments. Actual applications to MRS and the most recent advances: field gradients, diffusion, medical and biological applications, MRS in solids. The MRS of the future: The third dimension, minituarisation and the integration of other techniques. Practical component of the course.

Laboratory practicals:

STUDY PROGRAMME

Determination of the pulse at 90º. Homonuclear decoupling: double irradiation coherent in simple $^{1}H/^{1}H$ systems. Heteronuclear decoupling: double irradiation incoherent in simple $^{1}H/^{31}P$ systems. Solvent signal suppression (water). Dynamic ^{1}H MRS. DMF at variable temperatures, Tª of coalescence. ^{13}C MRS : Comparative study on a single sample of ^{13}C MRS, $^{13}C\{^{1}H\}$ MRS, DEPT-135. Simplification of couplings by an increase in the magnetic field. ^{1}H MRS of a 2.6-disubstituted pyridine ring in 400 MHz and 80 MHz apparatus. Determination of couplings to metallic centre through satellites in 400 MHz and 80 MHz apparatus. Temperature calibration using ^{1}H MRS: low temperature with methanol in MeOH-d_4, high temperature with 1.2-ethanodiol in DMSO-d_6. Isotopic effect on chemical displacement and the multiplicity of signals demonstrated by using ^{13}C MRS: $CHCl_3$ and $CDCl_3$, CH_2Cl_2 and CD_2Cl_2, acetone and acetone-d_6. Separation of methylene signals in an alcohol (pentanol or higher) using ^{1}H MRS: Alternative reactives. Determination of the excess enantiomeric of a mixture of enantiomeres using ^{1}H MRS: chiral markers, chiral solvating agents. Determination of the enantiomeric purity of alcohols using ^{31}P MRS: Use of an achiral auxiliary reagent as the PCl_3. Use of heteronuclei in the determination of enantiomeric purity: ^{59}Co MSR for $[Co(en)_3]Cl_3$. 2D experiments of variable complexity on relatively simple substrates: Ethanol, propanol, TMED, glutamic acid, … determination of couplings, coupling constants, connectivities and assignment of signals using COSY, HETCOR, 1D and 2D-INADEQUATE, and HSQC or HMQC. Determination of thermodynamic constants and of equilibrium through observation of heteronuclei, Schlenck equilibrium.

Unit 2. Molecular magnetism.

Theoretical:

Introduction to molecular magnetism (magnetization and magnetic susceptibility). Molecules with a single magnetic centre (without orbital momentum, with orbital momentum, spin transitions). Dinuclear compounds (isotropic interaction: radicals, Cu^{II} ions, other homodinuclear compounds; heteronuclear compounds; orbital models; magneto-structural correlations; the influence of dipolar, anisotropic and antisymmetric interactions). Oligonuclear (tri-, tetra-, etc.) compounds. 1D, 2D, 3D systems. Mixed-valence compounds.

Practicals:

Data fits given by χ_M vs T and $\chi_M T$ vs T curves to obtain the value of J in homo- and heterodinuclear systems of S = ½ ions, dinuclear S > ½ sytems, trinuclear systems and extended systems.

Unit 3. Electron-paramagnetic-resonance spectroscopy (EPR).

Theoretical:

Introduction to electron paramagnetic resonance (basic aspects of the technique, compounds that may be studied, signal types and how they are measured). The g-tensor (significance, anisotropic origin, casuistics of paramagnetic radicals and ions). Hyperfine and superhyperfine coupling. Fine structure (zero-field splitting). Chromophore systems with coupled electronic spin. Experimental aspects, limitations, fields of application and new tendencies.

Practicals:

Simulation of EPR spectra of samples in polycrystalline powder and solution (at both room and low temperatures): g and A parameters and the detection of zero-field splitting. The use of radical traps in EPR experiments. Oxidation-reduction reactions of biological interest: glutathione-induced reduction of Cu^{II} to Cu^{I}.

METHODOLOGY

The concepts and theoretical ideas will be interspersed with practical examples. The course will include some practical sessions to be conducted on the equipment and

instruments available with the help of the laboratory technician as well as on computers using the standard software.

BIBLIOGRAPHY

Basic reference works

1. H. Günther, "*NMR Spectroscopy. Basic Principles, Concepts, and Applications in Chemistry*", 2ª Ed., John Wiley & Sons, Nueva York, 1996.
2. H. Friebolin, "*Basic One and Two Dimensional NMR Spectroscopy*", 3ª Ed., VCH Publishers, Weinheim, 2004.
3. S. Braun, H. O. Kalinowski, S. Berger, "*200 and More NMR Experiments: A Practical Course*", 3ª Ed., VCH Publishers, Weinheim, 2004, (first edition 1996, second edition 1998).
4. J. J. Giménez Martínez, J. M. Expósito López, "*RMN Para Químicos Orgánicos*", Servicio de publicaciones de la Universidad de Almería, Almería, 1998.
5. U. Weber, H. Thiele, "*NMR Spectroscopy: Modern Spectral Analysis. Spectroscopic Techniques: An Interactive Course*", Wiley-VCH, Weinheim, 1998.
6. K. Itoh, M. Kinoshita, "*Molecular Magnetism: New Magnetic Materials*", Kodansha and Gordon & Breach, Tokyo-Amsterdam, 2000.
7. O. Kahn, "*Molecular magnetism*", VCH Publishers, Weinheim, 1993.
8. R. L. Carlin, "*Magnetochemistry*", Springer-Verlag, Berlin, 1986.
9. J. R. Pilbrow, "*Transition ion electron paramagnetic resonance*", Oxford University Press, Oxford, 1991.
10. J. A. Weil (Ed.), "*Electron paramagnetic resonance: elementary theory and practical applications*", John Wiley & Sons Inc., New York, 1998.
11. A. Bencini, D. Gatteschi "*Electron paramagnetic resonance of exchange coupled systems*", Springer-Verlag, New York, 1990.
12. F. E. Mabbs, D. Collison, "Electron Paramagnetic Resonance of d Transition Metal Compound", Elsevier, Amsterdam, 1992.

Other bibliographic works to consult

23. J. K. M. Sanders, B. K. Hunder, "*Modern NMR Spectroscopy. A Guide for Chemists*", 2ª Ed., Oxford University Press, Nueva York, reprinted in 1997.
24. K. M. Sanders, E. C. Constable, B. K. Hunder, C. M. Pearce, "*Modern NMR Spectroscopy. A Workbook of Chemical Problems*", 2ª, Ed., Oxford University Press, Nueva York, reprint of 1995.
25. K. Nakanishi (Ed.), "*One Dimensional and Two Dimensional NMR Spectra by Modern Pulse Techniques*", University Science Books, Mill Valley, 1990.
26. J. S. Miller, M. Drillon (Ed.), "*Magnetism: Molecules to Materials*", Wiley-VCH, Weinheim, 2001-2004. (Vols. I–V).
27. P. Day, A. E. Underhill (Ed.), "*Metal-Organic and Organic Molecular Magnets*", Royal Society of Chemstry, London, 2000.
28. W. Linert, M. Verdaguer (Ed.) "*Molecular magnets: recent highlights*", Springer-Verlag, Vienna, 2003.
29. F. Gerson, "*Electron spin resonance spectroscopy for organic radicals*", Wiley-VCH, Weinheim, 2003.
30. B. C. Gilbert, M. J. Davies, D. M. Murphy, K. A. McLauchlan, "*Electron paramagnetic resonance*" (antes "*Electron spin resonance*"), Royal Society of Chemistry, London, 2004. (Vol. XIX).
31. C. P. Poole, H. A. Farach, "*Handbook of electron spin resonance*", Springer-Verlag, New York, 1994-1999. (Vols. I-II).
32. C. P. Poole, "*Electron spin resonance: a comprehensive treatise on experimental techniques*", 2ª Ed., "Burgos- New York" 1997.

INTERNET RESOURCES
http://www.chem.queensu.ca/eprnmr/index.htm http://www.molmag.de/ http://msmd.ims.ac.jp/molspin/03mokuteki_e.html

ASSESSMENT
Methodology
Personalised follow up of each student will monitor progress throughout the course, the extent to which concepts are assimilated, and the student's capacity to put these into practice in an effective manner. To do so, reference will be made to the resolution of exercises, practical cases, seminars, tutorials, simulations and adjustments, theoretical-practical sessions using the equipment, and other activities.
Marking criteria
To this end, the work of the student will be assessed during for the theoretical part (30%). This percentage will include: active participation (20 %), questions formulated and responses given (10%). Likewise, the set theoretical-practical cases will be assessed (30%), and the student's performance during the practical part of the course (10%). Finally, the results of the evaluation tests will make up 30% of the global mark.

PROGRAMMED ACTIVITIES (Course contents and time frame)

Contents	Lecturer/s in charge	Hours	
		Taught Classes	Private study
Unit 1.-	Rafael Aguado	33	13
Unit 2.-	Luis Mª Lezama	14	9
Unit 3.-	Javier García	33	13
Exam preparation.		--	5
Completion of final assessment test		5	--
Total	**125**		

MASTER's DEGREE IN ADVANCED CHEMISTRY

POSTGRADUATE DEGREE IN ADVANCED CHEMISTRY
DEPARTMENT OF CHEMISTRY
FACULTY OF SCIENCES

UNIVERSITY OF BURGOS

COURSE			CODE
ADVANCED TECHNOLOGIES IN INDUSTRIAL PROCESSES			5254
Title	Centre		
MASTER's DEGREE IN ADVANCED CHEMISTRY	FACULTY OF SCIENCES		
Cycle	Semester	Nature	Num. of credits (T/P)
Second	1	Semi-optional	5 (3/2)

LECTURER (1) IN CHARGE OF THE COURSE			
José Luis Cabezas Juan			
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LECTURER (2)			
Sagrario Beltrán Calvo			
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LECTURER (3)			
Isabel Escudero Barbero			
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LECTURER (4)
Victorino Diez Blanco

Institution/firm	University of Burgos	Centre	Faculty of Sciences
Department	Biotecnology and Food Science	Area	Chemical Engineering
Office	Tel. num. (Ext.)	Email	
Area	8809	vdiezb@ubu.es	

STUDENT WORKLOAD		HOURS	
		Weekly	Total
TAUGHT CLASSES	Attendance at lectures	32 h/15 wks	32 h
	Attendance at practical classes (laboratory or computer room)	16 h/15 wks	16 h
	Attendance at seminars and activities	8 h/15 wks	8 h
	Attendance at assisted tutorials	8 h/15 wks	8 h
	Presentation of assignments	4 h/15 wks	4 h
	Completion of assessment tests	5 h/15 wks	5 h
PRIVATE STUDY	Group work for theoretical and/or practical classes.	16 h/15 wks	16 h
	Study for the preparation of theoretical and/or practical classes.	8 h/15 wks	8 h
	Resolution of exercises and practical cases, preparation of reports and presentations	12 h/15 wks	12 h
	Exam preparation.	16 h/15 wks	16 h
Total hours (Taught Classes)	73	**Total hours (Private Study)**	52
Total hours (Taught Classes and Private Study)	125		

COURSE CONTENTS (DESCRIPTORS)

- Supercritical fluid processes
- Membrane separation processes.
- Biological processes.
- Energy exploitation processes.

PREREQUISITES AND/OR PRIOR RECOMMENDATIONS

It is recommended that the student possess a basic knowledge at graduate level of mathematics, physics and chemistry.

OBJECTIVES

General

The student is expected to acquire sufficient understanding, based on a knowledge of processes in the Chemical Industry, to approach the study of the new technologies used in these processes and to perceive the improvements they have brought about.

Specific

To understand the fundamentals of the processes that use supercritical fluids. To develop the skills needed to operate with high pressure equipment.
To understand the scientific basis of membrane separation operations, the equipment that is used and to develop the skills needed to draft a report on a process that uses this technology.
To understand the scientific basis of bioprocesses, their current applications, the

equipment that is used and to develop the skills needed to draft a report on a process that uses this technology.
To understand energetic problems in industry, the scientific basis of energetic technology, its application to heat networks and cogeneration systems and to develop the skills needed to draft a report on a process which outlines an energy exploitation system.

SPECIFIC COMPETENCES (SKILLS AND KNOWLEDGE)

Unit 1
An understanding of the physical and thermodynamic properties of compressed fluids, particularly supercritical fluids, and of the mixtures in which they intervene.
An understanding of the fundamentals of the processes in which compressed fluids play a key role.
Knowledge of the process parameters and their influence in the performance of the processes that are carried out with compressed fluids.
Knowledge of the particularities and specific safety measurements of working with high pressure equipment.
The modelling of a process with simple models and the search for the design parameters to scale up the process.
Ability to describe actual industrial processes in which compressed fluids play a key role.
Unit 2
Ability to describe the principal membrane technologies and their most relevant characteristics.
Knowledge of the engineering fundamentals upon which the calculation of these operations are based.
Ability to describe present-day applications of membrane technology.
Knowledge of the operation of industrial equipment and its control variables.
Ability to develop working skills in the laboratory and for data analysis and treatment.
Knowledge of the main membrane manufacturers at present and the most common membrane modification techniques.
Ability to value the cost of an operation.
Ability to analyse practical cases and comment on solutions.
Unit 3
Capability to present bioprocess engineering principles involved in production processes as well as in environmental control in the chemical industry.
Ability to explain the essential mathematical models for the understanding and the design of biological processes.
Application of computer simulation programmes in the design and control of bioprocesses.
Unit 4
Students will develop an awareness of the need for energy and the problems that arise from energy consumption.
They will expand their knowledge of thermodynamic processes in which energetic transformations occur and learn about technological solutions to improve efficiency in industrial processes.
Students will gain an understanding of energy saving and the benefits of cogeneration and will learn about different types of renewable and non-renewable energies.
They will gain an understanding of the energetic situation in the chemical industry and of measures to exploit energy in the different industrial sectors.

GENERIC COMPETENCES (INSTRUMENTAL, INTERPERSONAL AND ORGANISATIONAL).

- Ability to search for information on a particular matter and use bibliographic

resources and information sources effectively.
- Acquire psychomotor skills in different experimental techniques and working methods used in technology transfer and research.
- Develop an ability to decide on the viability of a particular technological application that uses compressed fluids, membrane operations, bioprocesses and those directed at energy exploitation, and to distinguish those in which such processes would be neither viable nor competitive.
- Ability to assess the convenience of starting a research project on a concrete application in these fields and to develop such research.
- Understand and operate a membrane separation and bioprocessing SFE (extraction supercritical fluids) pilot plant.
- Interpret the results of any monitoring of these processes.
- Encourage favorable attitudes towards team work.
- Clearly express a position and a personal opinion on topics and problems discussed in the group.
- Acquire a critical vision of industrial processes and take a stance on the study and implantation of processes that use clean technologies and energetic efficiency.
- Learn to contrast opinions and to be receptive to constructive criticism.
- Information research and retrieval skills.
- Summary skills in order to prepare and present reports.

STUDY PROGRAMME

Unit 1. PROCESSES THAT USE SUPERCRITICAL FLUIDS.

Topic 1. Properties of compressed fluids and of mixtures with sub or supercritical components.

What is a supercritical fluid? PVT behaviour. Thermodynamic properties. Transport properties. Surface tension. Compressed fluids as solvents. Phase equilibrium. Experimental determination of phase equilibrium. Correlation and calculation of phase equilibria in binary and multi-component systems.

Topic 2. Supercritical fluid extraction.

Extraction of substances from solid substrates: Description of the process, Course of the extraction, Influence of process parameters and the conditions of the solid substrate on the extraction process, Modelling the Extraction, Applications. Solvent cycle: Separation of solvent and dissolved substances. Counter-current multistage extraction: Basic considerations, Process modelling, Practical cases.

Topic 3. Supercritical fluid particle formation.

Fundamentals of particle precipitation. Rapid Expansion of Supercritical Solutions (RESS). Particles from Gas Saturated Solutions (PGSS). Particle precipitation processes with a gas as the antisolvent: Gas antisolvent (GAS), Supercritical fluid antisolvent (SAS), Precipitation with compressed antisolvent (PCA), Solution enhanced dispersion by supercritical fluids (SEDS).

Topic 4. Concentration by adsorption processes in supercritical fluids.

Adsorbents. Solvents. Kinetic aspects. The effect of operational variables. Application to concentrations of essential oil on activated carbon.

Topic 5. Reactions in supercritical fluids.

Enzymatic reactions. Enzymes: Stability, effect of pressure, temperature and humidity. Enzyme inhibition. Chemical reactions. Types of reactors. Applications.

Topic 6. High-pressure equipment

Norms for the construction of high-pressure equipment. High-pressure recipients. Pressure-transfer equipment. Tubes, valves and accessories. Pilot plants and industrial equipment. Safety in process plants operating at high pressure. Risk identification. Reduction of risk in design, operation and maintenance. Legislation, norms and design

codes.

Practical programme
Practical 1: Visualization of the elements, the structure and the operation of a supercritical fluid extraction plant with solvent recirculation and of a dynamic analytical equipment to determine the solubility of solids in fluids.
Practical 2: Simulation of a supercritical fluid extraction process.

UNIT 2MEMBRANE SEPARATION PROCESSES.
Topic 1 – Introduction: Characteristics of membrane separation processes. Comparison with other separation processes. A history of the technology, present situation and future perspectives.
Topic 2 – Membrane materials: Commercial materials. Characterisation of structural parameters. Modification techniques:
Topic 3 – Operational designs: Fundamental aspects of transport. Factors that affect diminishing levels of fluid. Calculation methods and operational optimization of microfiltration, ultrafiltration, nonofiltration, inverse osmosis and electrodialysis.
Topic 4 – Cutting-edge technology: Separation of gases. Pervaporation. Liquid membranes. Dialysis. Membrane distillation. Thermo-osmosis. Other operations under investigation.
Topic 5 – Industrial applications: The pharmaceutical industry. The food industry. The chemical industry. Membrane reactors.

Unit 3. BIOPROCESSES
Biological processes in the chemical industry.
Estequiometry and the kinetics of biological reactions: growth, production and consumption.
Interactions between mass transfer and biological reaction.
Bioreactor design.
The operational modes of a bioreactor.
Monitoring and control.
Sterilization

Practicals
Use of the SuperPro Designer® and ASIM programmes in the design and simulation of an activated sludge bioreactor for wastewater treatment.
Practicals 3:
Use of the SuperPro Designer® and ASIM programmes in the design and simulation of an activated sludge bioreactor for the treatment of wastewaters.

Unit 4. TECHNOLOGIES AND ENERGY EXPLOITATION IN THE I.Q.
Topic 1 – Introduction to energetic technology: Introduction. Energetic transformations. Exergy.
Topic 2 – Industrial steam generators.
Topic 3 – Industrial ovens.
Topic 4 – Heat exchangers
Topic 5 – Heat exchange networks
Topic 6 – Cogeneration: Technological aspects. Cogeneration with gas turbines. Cogeneration with water vapour turbines. Combined cycle cogeneration.
Topic 7 - Conventional energies as energetic resources: Power plants. Nuclear power plants. Hydro-power plants.
Topic 8 – Non-conventional energies as energetic resources: Solar energy. Wind power. Other renewable energies.
Topic 9 – Situation and energy exploitation of the different sectors of the chemical industry:

Production and rational use of energy in the I.Q. Manufacturing processes and positioning of energetic exchange elements. Application of technology for energetic saving and reduced environmental impact. Energetic exploitation of waste products.

Practicals
Seminar on problems.
Operation of simulation programmes on the technology under study and the integrated processes.
Visits to companies that use these technologies, especially those that have cogeneration systems.

METHODOLOGY

- Theoretical classes using the whiteboard and auxiliary devices.
- Participative classes,
- Seminars on practical case studies
- Demonstrations of equipment and development of experiments in the laboratory and data treatment.
- Resolution of questionnaires and problems to support the learning process in each topic.
- Forum and chat sessions,
- Research and commentary on bibliographic sources and interesting news items related to the topic.
- Personalised tutorials
- Preparation and presentation of reports
- Self-evaluation by topics.
- Satisfaction and topic evaluation questionnaires on the set activities.
- Final written exam:

BIBLIOGRAPHY

Basic reference works

Unit 1

- Bertuco, A. and Vetter, G. "High Pressure Process Technology: Fundamentals and Applications" Elsevier. Amsterdam. 2001
- Brunner, G. "Gas Extraction. An Introduction to Fundamentals of Supercritical Fluids and the Application to Separation Processes" Steinkopff Darmstadt. Springer, New York. 1994.
- Brunner, G. "Supercritical Fluids as Solvents and Reaction Media" Elsevier. Amasterdam. 2004.
- King, C.J. "Separation Proceses". Editorial McGraw-Hill Book Company. New York. 1980
- Martínez, E. and Galán, M. A. "Extracción con fluidos supercríticos.(I). Fundamentos. Ingeniería Química". 1990, July , 169-175.
- McHugh M and V Krukonis. "Supercritical Fluid Extraction. Principles and Practice". Butterworth-Heinemann.Stoneham. MA. 1994. 2nd edition.
- King, M.R. and Bott. R.R. "Extraction of Natural Products using near critical Solvents". Blackie Academic. 1993
- Jessop P.G. and Leitner W. Eds. "Chemical Synthesis Using Supercritical Fluids". Wiley-VCH. 1999
- Kiran, E. "Supercritical Fluid. Fundamentals and applications".Nato ASI. Blackie Academic 2000.

Unit 2:

- Baker, R. W.; Cussler, E. L.; Eykamp, W.; Koros, W. J.; Riley, R. L. And Strathmann, H. "Membrane Separation Systems, Recent Developments and Future Directions" Noyen, Park Ridge, N. J. (1991).
- Crespo, G. J.; Bèddeker, K. W. "Membrane Processes in Separation and Purification" Kluwer Academic Publishers, Dodrecht, The Netherlands (1994).
- Cheryan, M. "Ultrafiltration and Microfiltration Handbook" Technomic Publishing Company Inc., Lancaster, USA (1998).
- Davis, H R. "Membrane Handbook" Ho, W. and Sirkar (eds.) Van Nostram Renhold, New York (1993).
- Ho, W. W. S.; Sirkar, K. K. (Eds.), "Membrane Handbook" Chapman and Hall, New York (1992).
- Matsuura, T. "Synthetic Membranes and Membrane Separation Processes" CRC Press, New Yok (1994).
- Mulder, M. "Basic Principles of Membrane Technology" Kluwer Academic Publishing, Dodrecht (1991).
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- Osada, Y and Nakagawa, T. (Eds.), "Membrane Science and Technology" Marcel Dekker, Inc. New York (1992).
- Rautenbach, R "Membrane Separation Processes" John Wiley. New York (1988).
- Scott, K. And Hughes R. "Industrial Membrane Separation Technology" Blackie Academic and Professional (1996).
- Wagner, J. "Membrane Filtration Handbook" Wagner Publishing, Gentofte, Denmark (1996).

Unit 3:

- Atkinson, B. "Reactores Bioquímicos". Reverté. Barcelona (1986).
- Bailey, J.E.; Ollis, D.F. "Biochemical Engineering Fundamentals". 2a ed. McGraw-Hill. New York (1986).
- Doran, P.M. "Principios de ingeniería de los bioprocesos". Editorial Acribia. Zaragoza. (1998).
- Coulson, J.M.; Richardson, J.F.; Backhurst, J.R.; Harker, J.H.; Peacock, D.G.; Sinnott, R.K. "Ingeniería Química. Diseño de Reactores Químicos, Ingeniería de la Reacción Bioquímica, Control y Métodos de Cálculo con Ordenadores" 2ª ed. Reverté. Barcelona (1984).

Unit 4:

- Bermúdez, V. "Tecnología energética" Servicio de Publicaciones de de la Universidad Politécnica de Valencia (2000)
- Sala Lizarraga, J.M. "Cogeneración. Aspectos termodinámicos, tecnológicos y económicos" Universidad del Pais Vasco (1999)
- Jiménez Gutierrez, A. "Diseño de procesos en ingeniería química" Ed. Reverté, Barcelona (2003)
- Manuales de Energías Renovables, IDEA, Madrid
- Situación Energética en la Industria, Centro de Estudios de la Energía, Ministerio de Industria, Madrid.

Other bibliographic works to consult

Unit 1

- Journal of Supercritical fluids

Unit 2

- Journal of Membrane Science

Unit 3

- Atkinson, B. "Reactores Bioquímicos". Reverté. Barcelona (1986).

- Bailey, J.E.; Ollis, D.F. "Biochemical Engineering Fundamentals". 2a ed. McGraw-Hill. New York (1986).
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- Coulson, J.M.; Richardson, J.F.; Backhurst, J.R.; Harker, J.H.; Peacock, D.G.; Sinnott, R.K. "Ingeniería Química. Diseño de Reactores Químicos, Ingeniería de la Reacción Bioquímica, Control y Métodos de Cálculo con Ordenadores" 2nd ed. Reverté. Barcelona (1984).

Unit 4:

- www.idae.es
- www.aven.es
- www.energuia.es
- www.enervia.es
- www.cores.es
- www.ree.es

INTERNET RESOURCES

Unit 1

- http://www.nottingham.ac.uk/supercritical/scintro.html: Visualisation across the saturation curve of the evolution of a substance when pressure and temperature are modified.
- http://www.supercriticalfluids.com/REAL-56k-Modem.rm: Video which shows a small quantity of naphthalene dissolved in SC-CO2 that changes from a clear solution to a cloudy speck as the pressure drops below the solubility curve. When the pressure rises again, the solution once again becomes clear when the naphthalene is dissolved in SC-CO2.
- http://www.chem.leeds.ac.uk/People/CMR/criticalpics.html: Images of a substance when two phases (liquid + vapour) form and when it has entered a supercritical phase.
- http://www.uigi.com/carbondioxide.html: specific information on carbon dioxide, its properties and uses.
- http://www.ceic.unsw.edu.au/centers/scf/scf_fig1.htm: summary on supercritical fluids: their properties and applications
- UBU E-campus platform within the virtual campus (UBUNet)

Unit 2

- www.membranes.com
- www.pcimem.com
- www.mempro.com
- www.pall.com
- www.kochmembrane.com
- www.ceramem.com
- www.membrana.es
- www.tami-industries.com

ASSESSMENT

Methodology

- Assessment of participation in taught classes.
- Active participation in the seminars and the laboratory practicals.
- Participation in the discussion for a created by the teacher.

- Self-evaluation tests by topics.
- Guidance and advice in the assisted tutorials.
- Bibliographic searches, capacity to analyse and to summarise.
- Preparation and presentation of the academic assignments.
- Participation in satisfaction and topic evaluation questionnaires on the set activities.
- Final written exam:

Marking criteria

Continuous assessment will be conducted through an evaluation of progress in the different set activities throughout the course. The following will be assessed:

- Attendance and participation in the taught classes that are programmed (20 %)
- Short questionnaires set on each topic (30%).
- At the end of each unit, the structure, development and presentation of a process of particular interest to be made by each student will be evaluated (30 %).
- Likewise, each student's ability to understand and operate a plant with the technology studied in each unit and to determine the elements needed for its design will be evaluated (20 %)

Other types of tests:

- If the assessment set out under the general criteria is not positive, a partly oral and partly written test will be set in which the student will demonstrate his/her knowledge of the course material (100%).

PROGRAMMED ACTIVITIES (Course contents and time frame)

Contents	Lecturer/s in charge	Hours	
		Taught Classes	Private study
Unit 1.			
Attend and participate actively in lectures and directed discussions	Sagrario Beltrán Calvo	7	
Laboratory practices and simulation	Sagrario Beltrán Calvo	4	
Attend and participate in seminars and on the resolution of practical cases	Sagrario Beltrán Calvo	4	
Tutorial assistance to resolve doubts and facilitate information and guidance	Sagrario Beltrán Calvo	2	
Assistance and participation in the presentation of prepared assignments	Sagrario Beltrán Calvo	1	
Completion of the assessment test	Sagrario Beltrán Calvo	1.25	
Group work with students for the practical assignments	Sagrario Beltrán Calvo		4
Private study to assimilate the material presented in theoretical and practical classes	Sagrario Beltrán Calvo		2
Resolution of exercises for seminars, preparation of reports and presentations	Sagrario Beltrán Calvo		3
Exam preparation.	Sagrario Beltrán Calvo		4
Unit 2.			

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught Classes	Private study
Attend and participate actively in lectures and directed discussions	Isabel Escudero Barbero	8	
Laboratory practices and simulations	Isabel Escudero Barbero	2	
Attend and participate in seminars and in the resolution of practical cases	Isabel Escudero Barbero	2	
Tutorial assistance to resolve doubts and facilitate information and guidance	Isabel Escudero Barbero	2	
Assistance and participation in the presentation of prepared assignments	Isabel Escudero Barbero	1	
Completion of the assessment test	Isabel Escudero Barbero	1.25	
Group work with students for the practical assignments	Isabel Escudero Barbero		4
Private study to assimilate the material presented in theoretical and practical classes	Isabel Escudero Barbero		2
Resolution of exercises for seminars, preparation of reports and presentations	Isabel Escudero Barbero		3
Exam preparation.	Isabel Escudero Barbero		4
Unit 3.			
Attend and participate actively in lectures and directed discussions	Victorino Diez Blanco	9	
Laboratory practices and simulation	Victorino Diez Blanco	4	
Attend and participate in seminars and in the resolution of practical cases	Victorino Diez Blanco	3	
Tutorial assistance to resolve doubts and to provide information and guidance	Victorino Diez Blanco	2	
Assistance and participation in the presentation of prepared assignments	Victorino Diez Blanco	1	
Completion of the assessment test	Victorino Diez Blanco	1.25	
Group work with students for the practical assignments	Victorino Diez Blanco		4
Private study to assimilate the material presented in theoretical and practical classes	Victorino Diez Blanco		2
Resolution of exercises for seminars, preparation of reports and presentations	Victorino Diez Blanco		3
Exam preparation.	Victorino Diez Blanco		4
Unit 4.			
Attend and participate actively in lectures and directed discussions	José Luis Cabezas Juan	8	
Laboratory practices and simulation	José Luis Cabezas Juan	2	

PROGRAMMED ACTIVITIES (Course contents and time frame)			
Contents	Lecturer/s in charge	Hours	
		Taught Classes	Private study
Attend and participate in seminars and in the resolution of practical cases	José Luis Cabezas Juan	3	
Tutorial assistance to resolve doubts and provide information and guidance	José Luis Cabezas Juan	2	
Assistance and participation in the presentation of prepared assignments	José Luis Cabezas Juan	1	
Completion of the assessment test	José Luis Cabezas Juan	1.25	
Group work with students for the practical assignments	José Luis Cabezas Juan		4
Private study to assimilate the material presented in theoretical and practical classes	José Luis Cabezas Juan		2
Resolution of exercises for seminars, preparation of reports and presentations	José Luis Cabezas Juan		3
Exam preparation.	José Luis Cabezas Juan		4