

**COURSE DESCRIPTION****1. Program data**

1.1 Higher education institution	“ALEXANDRU IOAN CUZA” UNIVERSITY OF IASI
1.2 Faculty	CHEMISTRY
1.3 Department	DOCTORAL SCHOOL OF CHEMISTRY
1.4 Field of study	CHEMISTRY
1.5 Cycle of studies	PHD
1.6 Study program / Qualification	PHD IN CHEMISTRY

2. Discipline data

2.1 Discipline title	FUNDAMENTAL CONCEPTS AND RECENT DEVELOPMENTS IN CHEMISTRY – MODULE I						
2.2 Course Activity Holder	Prof. univ. dr. Ionel MANGALAGIU Prof. univ. dr. Aurel PUI						
2.3 Owner of seminar activities	Prof. univ. dr. Aurel PUI Prof. univ. dr. Gabi DROCHIOIU						
2.4 Year of study	I	2.5 Semester	1	2.6 Type of evaluation	C	2.7 Discipline regime	CC

* CC – Compulsory / OP – Optional

3. Total estimated time (hours per semester and teaching activities)

3.1 Number of hours per week	2	of which: 3.2 course	1	3.3. seminar	1
3.4 Total hours in the curriculum	28	of which: 3.5. course	14	3.6. seminar	14
Distribution of the time fund					hours
Study by textbook, course material, bibliography and others					20
Additional documentation in the library, on specialized electronic platforms and in the field					20
Preparation of seminars/laboratories, assignments, papers, portfolios and essays					20
Tutoring					4
Examination					4
Other activities					4
3.7 Total individual study hours					72
3.8 Total hours per semester					100
3.9 Number of credits					4

4. Preconditions (if applicable)

4.1 Curriculum	-
4.2 Competences	-

5. Conditions (if applicable)

5.1 Course Conduct	
5.2 Conduct of the laboratory	-

6. Specific competences accumulated

Professional skills	To conceive and carry out original research, based on advanced methods that lead to the development of scientific, technological knowledge and/or research methodologies. Critical-constructive evaluation of projects and results of scientific research, assessment of the state of theoretical and methodological knowledge; identifying the priorities of knowledge and application to the field Selection and application of principles, theories and advanced methods of knowledge, transfer of methods from one field to another, interdisciplinary approaches to solve theoretical and practical problems, new and complex.
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	<p>The use of advanced principles and methods for explaining and interpreting, from multiple perspectives, new and complex theoretical and practical situations/problems, specific to the field.</p> <p>Systematic, advanced knowledge of concepts, research methods, controversies and new hypotheses specific to the field; communication with specialists in related fields.</p>
Transversal competences	<p>Development of projects centered on creativity, as a basis for self-realization</p> <p>Assuming responsibility and capacity to organize and manage the activity of professional groups, scientific research or organizations/institutions</p> <p>Initiation and innovative development of complex theoretical and practical projects</p>

7. The objectives of the discipline (from the grid of specific skills accumulated)

7.1. General objectives	<p>The course aims to highlight, starting from the fundamental concepts, what are the current trends in the research carried out by the academic team within the doctoral school of chemistry. The elements of novelty and scientific progress in the field of chemistry will be highlighted, both in relation to the specialized literature and in relation to the results obtained by the doctoral supervisors within the doctoral school of chemistry</p>
7.2. Specific objectives	<p>Cognitive objectives</p> <ul style="list-style-type: none">• Competences in identifying, developing and elaborating possible research topics. <p>Procedural objectives</p> <ul style="list-style-type: none">• Competences in the development of review articles for a given topic.• Knowing the research potential of the doctoral supervisors of the doctoral school of chemistry. <p>Attitudinal objectives</p> <ul style="list-style-type: none">• Correct use of fundamental concepts in relation to current trends in chemistry to achieve excellence in research.

8. Content

8.1	Course	Teaching methods	Observations (hours, bibliographic references, procedure)
1.	Advanced NMR methods and applications. The influence of molecular symmetry and chirality on proton magnetic resonance spectra	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [1÷2]) C-CF&TAC-01
2.	Two-dimensional nuclear magnetic resonance spectroscopy. Principles of two-dimensional NMR spectroscopy. Graphical presentation of the two-dimensional NMR spectra.	Lecture, Explanation, Conversation, Description, Problematization	(2 hour, [1÷2]) C-CF&TAC-02
3.	Spin-spin coupling constants and the Homonuclear Spin Echo experiment. Two-Dimensional Echo Spin Spectroscopy. Some experimental aspects of 2D-COSY spectroscopy	Lecture, Explanation, Conversation, Description, Problematization	(2 hour, [1÷2]) C-CF&TAC-03
4.	Organic retrosynthesis. Analysis of organic compounds with a single functional group obtained by retrosynthesis.	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [6]) C-CF&TAC-04
5.	Methods of synthesis of coordination compounds with organic ligands.	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [7,8]) C-CF&TAC-05



6.	Investigation of the structure of coordination compounds	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [7,8]) C-CF&TAC-06
7.	Theory of Sonochemistry. Trends in Sonochemistry	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [3-5]) C-CF&TAC-07
8.	Ultrasound assisted synthesis of new organic compounds. Synthesis of photoactive materials under ultrasound irradiations	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [3-5]) C-CF&TAC-08
9.	Ultrasonounds in combination with ionic liquids. Sonochemical reactors	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [3-5]) C-CF&TAC-09
10.	Microwaves in chemistry. Fundamentals of microwave chemistry	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [10,11]) C-CF&TAC-10
11.	Monomod and multimod reactors	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [10,11]) C-CF&TAC-11
12.	Applications of microwave in chemistry	Lecture, Explanation, Conversation, Description, Problematization	(1 hour, [10,11]) C-CF&TAC-12

Bibliography:

1. G. Roos, C. Roos. Organic Chemistry Concepts: An EFL Approach, Academic Press, **2014**;
2. H. Günther. NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry Wiley-VCH, **2013**;
3. Juan Carlos Colmenares, Gregory Chatel (eds.), Sonochemistry: From Basic Principles to Innovative Applications Series: Topics in Current Chemistry Collections, Springer International Publishing, **2017**;
4. J.L. Luche, C. Bianchi. Synthetic Organic Chemistry. Kluwer Publishers: Dordrecht, Netherlands, **1998**.
5. T.J. Mason. ed. Advances in Sonochemistry, vols. 1-5. JAI Press: New York, **1990, 1991, 1993, 1996, 1999**.
6. V. Sunjic, V. Perokovic, Organic Chemistry from Retrosynthesis to Asymmetric Synthesis, Springer, **2016**.
7. A.D.Garnovski, B. I. Kharisov, Direct Synthesis of Coordination and organometallic compounds, Elsevier, **1999**.
8. Ulrich Schbert, N. Husing, R. Laine (Editors), Materials Syntheses, A practical Guide, Springer Wien New York, **2008**.
9. D. W Bruce, D O'Hare, Inorganic Materials, John Wiley & Sons, **1997**.
10. A. Loupy . Microwaves in Organic Synthesis, Wiley, Weinheim, Germany, **2002, 2006**
11. O. C. Kappe, A. Stadler. Microwaves in organic and medicinal chemistry, Wiley, Weinheim, Germany, **2005**.

8.2	Seminar	Teaching methods	Observations (hours, bibliographic references, procedure)
1.	Two-dimensional nuclear magnetic resonance spectroscopy. Principles of two-dimensional NMR spectroscopy	Lecture, Explanation, Conversation, Description, Problematization	(2 hours, [1÷3]) S-CF&TAC-01
2.	Ultrasonounds assisted synthesis of new organic compounds	Lecture, Explanation, Conversation, Description, Problematization	(2 hours, [4,8]) S-CF&TAC-02
3.	3+n Dipolar cycloaddition reactions under ultrasonounds irradiations	Lecture, Explanation, Conversation, Description, Problematization	(2 hours, [4,8]) S-CF&TAC-03
4.	Organic retrosynthesis. Specific synthesis methods.	Lecture, Explanation, Conversation, Description, Problematization	(2 hours, [5]) S-CF&TAC-04
5.	FT-IR spectroscopy used in determining the structure of chemical compounds	Lecture, Explanation, Conversation, Description, Problematization	(2 hours, [3,7]) S-CF&TAC-05
6.	Ultrasonounds assisted synthesis of materials and organic compounds	Lecture, Explanation, Conversation, Description, Problematization	(4 hours, [5,8]) S-CF&TAC-06

Bibliography:

1. G. Roos, C. Roos, Organic Chemistry Concepts: An EFL Approach, Academic Press, **2014**;



- H. Günther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry Wiley-VCH, 2013.
- C.J. Pouchert, J. Behnche. The Aldrich Library of 13-C and 1-H FT NMR Spectra. Vol 1-3, Aldrich Chemical Company, Milwaukee, Wisconsin, USA 53210. ISBN 0-941633-34-9
- C. Oliver Kappe, D. Dallinger, S. Shaun Murphree. Practical Microwave Synthesis for Organic Chemists, Wiley, Weinheim, Germany, 2005.
- K. S. Suslick. Sonochemistry, in Kirk-Othmer Encyclopedia of Chemical Technology, 4th Ed. J. Wiley & Sons: New York, vol. 26, 517-541, 1998.
- V. Sunjic, V. Perokovic. Organic Chemistry from Retrosynthesis to Asymmetric Synthesis, Springer, 2016.
- R. Salzer, H. Siesler, Infrared and raman Spectroscopic Imaging, Wiley-VCH Verlag, 2009.
- Lucrari stiintifice 2000-2022 ptof.dr. Ionel I. Mangalagiu.

9. Corroborating the content of the discipline with the expectations of the representatives of the community, professional associations and representative employers in the field related to the program

After completing and advancing the discipline, the doctoral student will be able to identify a possible research topic and will be able to carry out a research project in a given topic based on a documented literature study

10. Rating

Activity Type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Weight in final grade (%)
10.4 Course	Correctness of answers – understanding and correct application of the issues dealt with in the course. The degree of assimilation of the specialized language	Colloquium – Lecture on a research ethics problem	75
10.5 Seminar	Correctness of answers – understanding and correct application of the issues dealt with in the seminar	Lecture on a topic discussed in the seminar	25
10.6 Minimum Performance Standard			
<ul style="list-style-type: none">Knowledge of the basic foundations for the topics of interest;The correct use of methods and techniques, materials, substances and equipment in compliance with occupational health and safety norms when performing a chemical experiment;The correct selection of the type of analysis method depending on the objective of the analysis.			

Date of completion

Course holder

Seminar holder

28.09.2022

Prof. univ. dr. Ionel MANGALAGIU

Prof. univ. dr. Aurel PUI

Prof. univ. dr. Aurel PUI

Prof. univ. dr. Gabi DROCHIOIU

Date of approval

Director of the Doctoral School of Chemistry
Prof. univ. dr. habil. Cecilia ARSENE