

## FIȘA DISCIPLINEI

### 1. Date despre program

1.1 Instituția de învățământ superior	Universitatea Babeș-Bolyai, Cluj-Napoca
1.2 Facultatea	Chemistry and Chemical Engineering
1.3 Departamentul	Chemistry
1.4 Domeniul de studii	Chemistry
1.5 Ciclul de studii	Master
1.6 Programul de studiu / Calificarea	MOLECULAR MODELING IN CHEMISTRY AND BIOCHEMISTRY/ Master's Degree

### 2. Date despre disciplină

2.1 Name of the discipline	<b>Advanced Organometallic Chemistry - CME6122</b>						
2.2 Course coordinator	Conf. Dr. Richard A. Varga						
2.3 Seminar coordinator	Conf. Dr. Richard A. Varga						
2.4 Year of study	I	2.5 Semester	2	2.6. Type of evaluation	E	2.7 Type of discipline	DF

### 3. Total estimated time (hours/semester of didactic activities)

3.1 Hours per week	4	Of which: 3.2 course	2	3.3 seminar/laboratory	2
3.4 Total hours in the curriculum	56	Of which: 3.5 course	28	3.6 seminar/laboratory	28
Time allotment:					ore
Learning using manual, course support, bibliography, course notes					25
Additional documentation (in libraries, on electronic platforms, field documentation)					20
Preparation for seminars/labs, homework, papers, portfolios and essays					15
Tutorship					5
Evaluations					4
Other activities: not the case					-
3.7 Total individual study hours	69				
3.8 Total hours per semester	125				
3.9 Number of ECTS credits	5				

### 4. Prerequisites (if necessary)

4.1 curriculum	<ul style="list-style-type: none"> <li>Not the case</li> </ul>
4.2 competencies	<ul style="list-style-type: none"> <li>Not the case</li> </ul>

### 5. Conditions (if necessary)

5.1 for the course	<ul style="list-style-type: none"> <li>Students will receive the course support.</li> <li>Interactive participation will be encouraged</li> <li>Students will turn off their mobile phones</li> </ul>
5.2 for the seminar / lab activities	<ul style="list-style-type: none"> <li>Students will turn off their mobile phones</li> <li>Students will attend the laboratory with coat, gloves, safety glasses</li> <li>Tardiness will not be accepted</li> </ul>

## 6. Specific competencies acquired

Professional competencies	<p><b>C1. Description, analysis and use of advanced concepts and theories in the field of chemistry</b></p> <ul style="list-style-type: none"> <li>• C1.1. Recognition and description of complex concepts, approaches, theories, methods and models regarding the structure and reactivity of chemical compounds</li> <li>• C1.2. Explanation and interpretation of properties, concepts, approaches, theories, models and fundamental notions of structure and reactivity of chemical compounds</li> <li>• C1.3. Application of fundamental concepts to solve problems associated with the structure and reactivity of chemical compounds</li> <li>• C1.4. Critical analysis of existing models and theories regarding the structure and reactivity of chemical compounds</li> <li>• C1.5. Development of projects about the structure and reactivity of chemical compounds through the lens of existing models and theories</li> </ul> <p><b>C2. Carrying out experiments with a high degree of difficulty, rigorously applying analysis methods and interpretation the results, in compliance with occupational health and safety regulations</b></p> <ul style="list-style-type: none"> <li>• C2.1. Identification of methods and techniques, materials, substances and equipment needed to perform experiments</li> <li>• C2.2. Strategy development, description and interpretation of high-difficulty laboratory experiments</li> <li>• C2.3. Carrying out laboratory experiments with a high degree of difficulty and interpretation of the obtained results</li> <li>• C2.4. Critical analysis and interpretation of how laboratory experiments are conducted and the results obtained</li> <li>• C2.5. Elaboration and presentation of a report on the conduct of a laboratory experiment with a description of the working method and interpretation of the results</li> </ul>
Transversal competencies	<ul style="list-style-type: none"> <li>• Permanent information and documentation in the field of activity</li> <li>• Self-evaluation of professional performances and establish the needs of continuous learning, documentation in the work fields in correlation to the labour market</li> <li>• The ability to write and defend reports.</li> </ul>

## 7. Objectives of the discipline (outcome of the acquired competencies)

7. General objective of the discipline	<ul style="list-style-type: none"> <li>• Assimilation of advanced knowledge of organometallic chemistry</li> <li>• acquisition of knowledge regarding general concepts (general properties, synthesis and reactivity); compounds of main group metals and transition metals; fluxional molecules; hypervalent compounds and metal-metal bonded compounds (including clusters); notions regarding applications in organic synthesis and catalysis; notions of structural analysis in organometallic chemistry.</li> </ul>
7.2 Specific objective of the discipline	<ul style="list-style-type: none"> <li>• the ability to synthesize organometallic compounds using direct synthetic methods or their chemical properties (reactivity)</li> <li>• knowledge about the synthesis of organometallic compounds in unusual oxidation states</li> <li>• the ability to use spectroscopic methods to establish the structure of organometallic compounds</li> <li>• the habit of working in a group, the ability to express oneself freely on a given topic, to use specialized literature, to prepare an essay/report on a given topic.</li> </ul>

## 8. Content

8.1 Lecture	Teaching methods	Remarks
<b>1. Introductory notions. Metal-carbon bond types - reactivity</b> (updating notions acquired in previous courses) (M-C bond, reactivity).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>2. General properties of organometallic compounds</b> (18-electron rule – limits).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>3. Oxidation states and coordination numbers in organometallic compounds</b> (oxidation state, metal-metal bond, coordination number).	Lecture; Explanation; Conversation; Problems	2 hours
<b>4. Organometallic compounds of Li and Na in organometallic synthesis</b> (reactivity, organolithium, organosodium).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>5. Organometallic compounds of Mg and Hg in organometallic synthesis</b> (reactivity, Grignard reagents, organomercury, mercury toxicity).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>6. Organometallic compounds with single metal-metal bond in compounds of main group metals - acyclic and cyclic systems</b> (single metal-metal bond, metallocycles).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>7. Organometallic compounds with multiple metal-metal bonds</b> (double and triple metal-metal bond).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>8. Organometallic clusters: metallocarbonyls - synthesis and properties</b> (clusters, metallocarbonyls, structural types, synthesis).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>9. Organoheterometallic clusters – synthesis and properties</b> (clusters, structural types, isolobality).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>10. Organometallic compounds of transition metals with <math>\sigma</math>-donor and <math>\sigma</math>-donor/<math>\pi</math>-acceptor ligands</b> (M-alkyl, M-aryl, kinetic and thermodynamic stability, M-carbenes, M-carbynes).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>11. Organometallic compounds of transition metals with <math>\pi</math>-donor/<math>\pi</math>-acceptor ligands</b> (M-olefin, M-alkyne, M-cyclopentadienyl, M-arene).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>12. Nuclear Magnetic Resonance (NMR) in the investigation of organometallic compounds. Fluxional molecules</b> (NMR active isotopes, metal-proton, metal-carbon couplings, dynamic character in solution, fluxional molecules).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>13. Hypervalent organometallic compounds – synthesis and structure</b> (hypervalence, stability, oxidation states, dynamic character).	Lecture; Explanation; Conversation; Description; Problems	2 hours
<b>14. Applications in organic synthesis and introduction in organometallic catalysis</b> (catalytic processes, C-nonmetal bond activation).	Lecture; Explanation; Conversation; Description; Problems	2 hours

## References

1. I. Haiduc, *Chimia compușilor organometalici*, Editura Stiintifica, Bucuresti, 1974.
2. Ch. Elschenbroich, *Organometallics - Third, Completely Revised and Extended Edition*, 3<sup>rd</sup> Ed., VCH Verlag, Weinheim, 2006.
3. R. H. Crabtree, *The Organometallic Chemistry of The Transition Metals*, 4<sup>th</sup> Ed., John Wiley & Sons, New York, 2005.

4. Suport de curs, prezentare PowerPoint.

**Optional references (the discipline holder's library):**

1. I. Haiduc, J. J. Zuckerman, *Basic Organometallic Chemistry*, Walter de Gruyter, Berlin, 1985.
2. S Komiya (Ed.), *Synthesis of Organometallic Compounds – A Practical Guide*, John Willey & Sons, Chichester, 1998.
3. I. Omae, *Applications of Organometallic Compounds*, John Willey & Sons, Chichester, 1998.
4. Kin-ya Akiba (Ed.), *Chemistry of Hypervalent Compounds*, Wiley-VCH, New York, 1999.
5. D. Morales-Morales, C. Jensen (Eds.), *The Chemistry of Pincer Compounds*, Elsevier, Amsterdam, 2007.
6. M. Bochmann, *Organometallics and Catalysis*, Oxford University Press, Oxford, 2014.
7. Parkin, G. Classification of Organotransition Metal Compounds. In *Comprehensive Organometallic Chemistry III*, Volume 1, Chapter 1; Crabtree, R. H. and Mingos, D. M. P. (Eds), Elsevier, Oxford, 2006.

8.2 Seminar / laboratory	Teaching methods	Remarks
<b>1. Techniques for the synthesis of sensitive organometallic compounds to open atmosphere (water, oxygen, carbon dioxide)</b> (reactivity, anhydrous solvents, manipulation of sensitive compounds).	Experiment; Explanation; Conversation; Description; Problems	2 hours
<b>2. Synthesis of an organolithium derivative under argon atmosphere</b> (organolithium compounds, Grignard reagent, structure, reactivity).	Experiment; Explanation; Conversation; Description; Problems	10 hours
<b>3. Syntheses of organometallic derivatives of non-transition metals in air and under argon atmosphere</b> (metathesis and redistribution reactions).	Experiment; Explanation; Conversation; Description; Problems	10 hours
<b>4. Analysis of the prepared organometallic compounds by NMR spectroscopy</b> (resonance signals, coupling constants, dynamic process).	Explanation; Conversation; Description; Problems	5 hours
<b>5. Colloquy.</b>	Test	1 hour

**9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program**

- By acquiring the theoretical-methodological concepts and approaching the practical aspects included in the **Advanced Organometallic Chemistry** discipline, students acquire consistent knowledge and will provide the students with the competencies requested by ANC.

**10. Evaluation**

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the final grade (%)
10.4 Course	Correctness of answers – proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within new contexts. Correct solving of the problems as part of the examination subjects	<ul style="list-style-type: none"> <li>• oral exam – access to the exam is conditioned by taking the laboratory colloquium and presenting laboratory reports corresponding to all practical works</li> <li>• Proven or intended fraud is punished according to the ECST rules of UBB.</li> <li>• <i>appeals</i> are resolved by the discipline holder</li> </ul>	80%
10.5 Seminar/	• Correctness of answers –	• the laboratory reports corresponding	20%

laboratory	proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within new contexts. <ul style="list-style-type: none"> <li>• the quality of the prepared reports</li> <li>• the activity carried out in the laboratory</li> </ul>	to all practical works - they will be delivered according to the schedule established at the beginning of the semester <ul style="list-style-type: none"> <li>• the exam will also contain questions related to experimental and laboratory activities</li> </ul>	
10.6 Minimum performance standards			
<ul style="list-style-type: none"> <li>• Nota 5 (cinci) atât la colocviul de laborator, cât și la examenul oral.</li> <li>• Grade 5 (five) both at the exam as well as colloquium</li> </ul>			

Date  
11.03.2024

Signature of course coordinator



Signature of seminar coordinator



Date of approval  
13.03.2024

Signature of the head of department

