COURSE DESCRIPTION

NMR and X-ray Diffraction in Organometallic Chemistry

Academic year 2025-2026

1. Programme-related data

1.1. Higher Education Institution	Babeș-Bolyai University
1.2. Faculty	Faculty of Chemistry and Chemical Engineering
1.3. Department	Doctoral School of Chemistry
1.4. Field	Chemistry
1.5. Level of study	PhD degree
1.6. Degree programme / Qualification	PhD degree
1.7. Form of education	With frequency

2. Course-related data

2.1. Course title	NMR and X-ray Diffraction in Organometallic Chemistry			Course code	**SDC-19-01**
2.2. Course coordinator	Acad. Prof. dr. Cristian SILVESTRU				
2.3. Seminar coordinator	Acad. Prof. dr. Cristian SILVESTRU				
2.4. Year of study	I	2.5. Semester	2	2.6. Type of assessment	Exam
2.7. Course status	Optional		2.8. Tipul disciplinei		Specialisation subject

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

3.1. Number of hours per week	3	of which: 3.2. course	2	3.3. seminar/ laboratory/ project	1
3.4. Total of hours in the curriculum	36	of which: 3.5. course	24	3.6 seminar/ laboratory	12
Time allocation for individual study (IS) and self-taught activities (ST)					**hours**
Learning from textbooks, course materials, bibliography, and notes (IS)					100
Additional research in the library, on subject-specific electronic platforms, and on-site					50
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays					40
Tutoring (professional guidance)					8
Examinations					6
Other activities [i.e.: two-way communication with the course coordinator]					10
3.7. Total hours of individual study (IS) and self-taught activities (ST)				**214**	
3.8. Total hours per semester				**250**	
3.9. Number of credits				**10**	

4. Prerequisites (where applicable)

4.1. curriculum-related	Not applicable
4.2 skills-related	Not applicable

5. Specific conditions (where applicable)

5.1. course-related	• Courses are held with access to the internet and databases • Students will have access to databases (subscribed databases by the faculty/university, central library) • Interactive participation will be encouraged • Students will come to class with their mobile phones turned off
5.2. seminar/laboratory-related	• Seminars are held with access to the internet and databases • Students will come to the seminar with their mobile phones turned off

6.1. Competencies resulting from the completion of the degree programme[1]

Professional competencies	
Competency code	**Competency**
PC1	Advanced expertise in chemistry and doctoral-level research topics
PC4	Planning, designing, and implementing an original scientific research project, in compliance with academic ethics and integrity
PC5	Applying and developing advanced research and analytical methods; critically interpreting data and formulating innovative solutions
Transversal competencies	
Competency code	**Competency**
TC2	Advanced scientific communication in Romanian and English; collaboration in interdisciplinary and multicultural settings
TC3	Advanced digital skills for research, data analysis, and dissemination; responsible use of digital tools.

6.2. Learning outcomes relevant to the degree programme (as referred to in the curriculum)[2]

Learning outcomes targeted by the subject		
Competency code	**Knowledge and comprehension**	**Specific academic skills**
PC1	Advanced and up-to-date knowledge in chemistry and the research field; critical understanding of the scientific literature.	Applies and synthesizes advanced concepts/theories to formulate research hypotheses; justifies the choice of scientific approaches.
PC4	Advanced research methodologies: experimental design, modern synthesis and characterization techniques, analysis and validation; principles of research project management.	Designs, plans and implements a research project; applies quality and safety procedures and documents stages and data with full traceability.
PC5	Advanced strategies for data analysis, interpretation, and integration; evaluation of methodological limitations, reproducibility, and scientific impact.	Critically analyses complex data, estimates uncertainty and formulates conclusions; proposes methodological improvements and directions for research/innovation.
TC2	Scientific terminology and communication in Romanian and English; the structure of scientific articles and presentations; good citation practices.	Writes and presents scientific results in Romanian/English coherently; provides well-argued responses to comments and peer reviews.
TC3	Digital tools for research, citation, and data processing (databases, specialized software, reference managers); responsible use of digital resources.	Uses discipline-specific digital tools effectively; manages citations; uses digital resources responsibly in research activities.

7. Subject-specific learning outcomes

Knowledge and understanding
1. Defining and acquiring the basic notions, concepts, theories and models used in structural analysis by Nuclear Magnetic Resonance (NMR) and specific Single Crystal X-Ray Diffraction and their appropriate use in professional communication.

[1] The professional and/or transversal skills targeted by the subject for which the course description is prepared will be copied from the curriculum of the degree programme. For each competency, the complete entry, including the competency code, will be copied with the exact wording that appears in the curriculum, without any changes. If no competency is copied from either of the two categories, the row corresponding to that category is deleted from the table.

[2] The learning outcomes relevant for the degree programme and targeted by the subject for which the course description is prepared will be listed. The entries, copied without any changes from the Curriculum by subject type (Core Subject/Specialisation Subject/Complementary Subject), are listed under the corresponding competency.

2.	Use of in-depth knowledge in the field of chemistry for the explanation and interpretation of NMR spectra, respectively the structural analysis of inorganic (including coordination) and organometallic compounds. Processing and interpretation of spectroscopic data.
3.	Developing the ability to determine the molecular structure in solution or solid state of inorganic, organic and organometallic compounds using data obtained from NMR spectra. Using NMR spectroscopy in solution in the study of dynamic systems (including fluxional).
4.	Ability to use structural data of inorganic (including coordination), organic and organometallic compounds, obtained by single crystal X-ray diffraction. Use of single crystal X-ray diffraction data in identifying aspects in the field of supramolecular chemistry.
5.	Use of specific software for processing NMR spectra and single crystal X-ray diffraction data.
6.	Ability to understand and interpret complementary data for the characterization of inorganic (including coordination), organic and organometallic compounds, to express and argue the interpretation of data based on the correlation of results and comparison with data from the specialized literature.
	Specific academic skills
1.	Performing the requested tasks according to the specified requirements and within the deadlines imposed, in compliance with the norms of professional ethics and moral conduct, following a pre-established work plan.
2.	Solving the requested tasks in accordance with the general objectives established by integrating into a working group.
3.	Permanent information and documentation, in Romanian and in an internationally spoken language, in its field of activity, using modern information and communication methods (specific software, database search).
4.	Concern about improving the results of professional activity through involvement in the activities carried out.
5.	Ability to prepare written papers and publicly defend these papers.

8. Contents

8.1 Course	**Teaching and learning methods**	**Remarks [3]**
8.1.1. Nuclear Magnetic Resonance - principle of the method; NMR active isotopes, internal and external standards, spectral parameters.	Lecture, explanation, conversation.	2 hours/week
8.1.2. Multinuclear NMR spectroscopy – ^{1}H, ^{13}C.	Lecture, explanation, conversation.	2 hours/week
8.1.3. Multinuclear NMR spectroscopy – ^{19}F, ^{31}P and other NMR active isotopes of nonmetals.	Lecture, explanation, conversation.	2 hours/week
8.1.4. Multinuclear NMR spectroscopy – NMR active isotopes of some metals; spin-spin coupling with nuclei with abundance 100% or less than <100% - satellites.	Lecture, explanation, conversation.	2 hours/week
8.1.5. NMR spectroscopy. Two-dimensional NMR.	Lecture, explanation, conversation.	2 hours/week
8.1.6. NMR spectroscopy – correlations between coordination geometry, number of signals and chemical shift in the spectra of inorganic and coordination compounds.	Lecture, explanation, conversation, description, problem.	2 hours/week
8.1.7. Fluxional molecules.	Lecture, explanation, conversation.	2 hours/week
8.1.8. NMR spectroscopy – dynamic NMR, kinetic and thermodynamic parameters.	Lecture, explanation, conversation, description, problem.	2 hours/week
8.1.9. Single crystal X-ray diffraction (principle of the method and instrumentation).	Lecture, explanation, conversation, description.	2 hours/week
8.1.10. Interpretation of data obtained by single crystal X-ray diffraction. Description and interpretation of cif files, crystallographic tables, atomic parameters. Covalent atomic radii, Van der Waals radii.	Lecture, explanation, conversation, description.	2 hours/week

[3] For example, organisational aspects, recommendations for students, specific aspects relating to the course/seminar, such as inviting experts in the field, etc.

8.1.11. Intra- and intermolecular interactions. Noncovalent interactions – hydrogen bonds, hydrogen-pi bonds, metal-pi, pi-pi stacking, metallophilic, etc.	Lecture, explanation, conversation, description, problem.	2 hours/week
8.1.12. Supramolecular architectures obtained by self-assembly.	Lecture, explanation, conversation, description.	2 hours/week

Bibliografie

1. H. Selye, *De la vis la descoperire*, Ed. Medicală, București, 1968.
2. M. S. Rădulescu, *Metodologia cercetării științifice*, Ed. Didactică și Pedagogică, București, 2006.
3. C. Enăchescu, *Tratat de teoria cercetării științifice*, Ed. Polirom, București, 2005.
4. Mehlich, F. Moser, B. van Tiggelen, L. Campanella, H. Hopf, *The Ethical and Social Dimensions of Chemistry: Reflections*, *Considerations, and Clarifications*, *Chem. Eur. J.* **2017**, *23*, 1210 – 1218.
5. R. E. Spier, *Science and Engineering Ethics, Overview* in *Encyclopedia of Applied Ethics*, (Ed.: R. Chadwick), 2nd Ed., Elsevier, London, 2012.
6. *Research ethics*, in http://www.en.wikipedia.org/wiki/research_ro
7. *Research methodology*, in www.en.wikipedia.org/wiki/research_methodology
8. *Asociația Ad astra – "Evaluarea cercetării științifice"*, revista *Ad Astra*, nr. 4/**2005**.
9. Legea nr. 206/2004 privind buna conduită în cercetarea științifică, dezvoltarea tehnologică și inovare.

Bibliografie opțională

10. I. Haiduc, *Cercetarea științifică din România în context internațional. Evoluții recente. Colaborări internaționale*, **Academica**, Anul XII, Nr. 2-3, Mai-iunie **2002**, p. 56-59.
11. I. Haiduc, *Aspecte etice ale cercetării științifice în chimie, biologie și medicină*, *Revista de Politica Științei și Scientometrie*, **2005**, *3(1)*, 37–42.
12. H. Frank, L. Campanella, F. Dondi, J. Mehlich, E. Leitner, G. Rossi, K. N. Ioset, G. Bringmann, *Ethics, Chemistry, and Education for Sustainability*, *Angew. Chem. Int. Ed.*, **2011**, *50*, 8482–8490.
13. R. R. Ernst, *The Responsibility of Scientists, a European View*, *Angew. Chem. Int. Ed.*, **2003**, *42*, 4434–4439.

8.2 Seminar	**Teaching and learning methods**	**Remarks**
8.2.1-2. Applications of NMR spectroscopy in the structural analysis of organometallic and coordination compounds. Use of specific software (MestRENova). Interpretation of ^{1}H and ^{13}C spectra – structural considerations based on ^{1}H and ^{13}C chemical shifts, the value of ^{1}H resonance signal integrals, spin-spin couplings from ^{1}H NMR spectra of organometallic compounds.	Explanation, conversation, description, problem.	2 hours / 2 weeks
8.2.3-4. Applications of NMR spectroscopy in the structural analysis of organometallic and coordination compounds. Interpretation of two-dimensional spectra. Assignment of ^{1}H and ^{13}C resonance signals.	Explanation, conversation, description, problem.	2 hours / 2 weeks
8.2.5-6. Interpretation of NMR spectra (^{19}F, ^{31}P, etc.) of inorganic and organometallic compounds. Assignment of structure in solution based on multinuclear NMR spectra. Simulation of NMR spectra.	Explanation, conversation, description, problem.	2 hours / 2 weeks
8.2.7-8. NMR applications in the study of dynamic processes. Spectra at variable temperature. Kinetic and thermodynamic parameters.	Explanation, conversation, description, problem.	2 hours / 2 weeks
8.2.9-10. Analysis and interpretation of single crystal X-ray diffraction data. Use of specific software (Diamond, Mercury, Platon, etc.) and specific databases (CSD, ICSD, etc.).	Explanation, conversation, description, problematization	2 hours / 2 weeks
8.2.11-12. Using specific programs to prepare data for publication.	Explanation, conversation, description, problematization	2 hours / 2 weeks

Bibliografie

1. *Instructions for autors* pentru redactarea de articole științifice sau alte texte de specialitate (capitole de cârti, proiecte de cercetare, etc.) (bibliografie pusă la dispoziția cursanților de către titularul de curs)
2. *Pachet de informații pentru competiții de proiecte* (bibliografie pusă la dispoziția cursanților de către titularul de curs)

9. Evaluation

Type of activity	9.1 Evaluation criteria[4]	9.2 Evaluation methods[5]	9.3 Percentage in the final grade
9.4 Course	Correctness of answers – correct acquisition and understanding of the issue addressed The way of thinking, the correctness and argumentation of the proposed solutions	Oral exam	60%
9.5 Seminar	The activity carried out at the seminar	Presentation of spectra and structures analysis	40%
9.6 Minimum standard for passing			
Grade 5 (five)			

10. SDG labels (Sustainable Development Goals)[6]

	○	Sustainable Development Generic Label

1 FĂRĂ SĂRĂCIE	2 FOAMETE „ZERO”	3 SĂNĂTATE ȘI BUNĂSTARE	4 EDUCAȚIE DE CALITATE	5 EGALITATE DE GEN	6 APĂ CURATĂ ȘI SANITAȚIE	7 ENERGIE CURATĂ ȘI LA PREȚURI ACCESIBILE	8 MUNCĂ DECENTĂ ȘI CREȘTERE ECONOMICĂ	9 INDUSTRIE, INOVAȚIE ȘI INFRASTRUCTURĂ
○	○	○	X	○	○	○	○	○

10 INEGALITĂȚI REDUSE	11 ORAȘE ȘI COMUNITĂȚI DURABILE	12 CONSUM ȘI PRODUCȚIE RESPONSABILE	13 ACȚIUNE CLIMATICĂ	14 VIAȚA ACVATICĂ	15 VIAȚA TERESTRĂ	16 PACE, JUSTIȚIE ȘI INSTITUȚII EFICIENTE	17 PARTENERIATE PENTRU REALIZAREA OBIECTIVELOR	No label applies
○	○	○	○	○	○	○	○	○

Date of entry:

January 30, 2026

Signature of course coordinator

Signature of seminar coordinator

Date of approval in CDSC:

Signature of the Director of the DSC

Prof. dr. Niculina Daniela Hădade

[4] The evaluation criteria must directly reflect the learning outcomes targeted at the level of the degree programme respectively at the level of the subject. More specifically, the learning outcomes set out in the expected learning outcomes are assessed.

[5] Both final evaluation methods and ongoing evaluation strategies should be established.

[6] Select a single label which, according to the *Implementation of SDG labels in the academic process*, best matches the subject. If the subject addresses sustainable development in a generic manner (i.e. by presenting/introducing the general framework of sustainable development, etc.), then the Sustainable Development generic label may be applied. If none of the labels describe the subject, select the last option: *"No label applies."*