COURSE DESCRIPTION

Stereochemistry and supramolecular chemistry

Academic year 2025-2026

1. Programme-related data

1.1. Higher Education Institution	Babes-Bolyai University
1.2. Faculty	Chemistry and Chemical Engineering
1.3. Department	Doctoral School of Chemistry
1.4. Field	Chemistry
1.5. Level of study	doctoral
1.6. Degree programme / Qualification	Doctorate in Chemistry/ Doctor in Chemistry
1.7. Form of education	Full Time

2. Course-related data

2.1. Course title	Stereochemistry and supramolecular chemistry			Course code	SDC-19-03
2.2. Course coordinator	Grosu Ion				
2.3. Seminar coordinator	Grosu Ion				
2.4. Year of study	I	2.5. Semester	II	2.6. Type of assessment	Exam
2.7. Course status	Optional			2.8. Course type	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)					60
Additional research in the library, on subject-specific electronic platforms, and on-site					60
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays					60
Tutoring (professional guidance)					24
Examinations					5
Other activities					5
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	-
4.2 skills-related	-

5. Specific conditions (where applicable)

5.1. course-related	-
5.2. seminar/laboratory-related	-

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

Professional competencies	
Competency code	**Competency**

[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.

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 comprehension
1. The student explains and integrates advanced concepts of stereochemistry, including symmetry elements and operations, point groups, chirality and enantiomerism, as well as the basic notions of diastereoisomerism and conformational analysis for acyclic and cyclic compounds
2. The student describes and interprets the fundamental principles of supramolecular chemistry, the nature and role of non-covalent interactions, general synthetic methods for macrocyclic and mechanically interlocked compounds, and their main physical and chemical properties, as well as the types of supramolecular architectures obtained by self-assembly
3. The student interprets the relationship between stereochemical structure (configurational and conformational) and physicochemical properties, optical activity, reactivity, and molecular recognition behaviour in host–guest systems and supramolecular architectures
4. The student correlates modern examples from the scientific literature on macrocycles, mechanically interlocked molecules, and adaptive supramolecular systems with the theoretical principles of stereochemistry and supramolecular chemistry, highlighting current research directions in the field
Specific academic skills

[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.

1. The student classifies stereoisomers (enantiomers, diastereoisomers, conformers), assigns configuration descriptors (R/S, E/Z and other descriptors where appropriate), and represents stereochemical structures using different formula types and molecular models (Fischer, Newman, spatial models, etc.).
2. The student applies conformational analysis and relevant spectroscopic methods (e.g. interpretation of NMR data) to deduce preferred conformations, rotational barriers, and structure–property relationships in acyclic compounds, cycloalkanes and heterocyclic systems.
3. The student critically uses the concepts of non-covalent interactions, molecular recognition and self-assembly to analyse and, at an introductory level, propose synthetic strategies and behavioural models for macrocyclic compounds, host–guest systems, self-assembled supramolecular architectures and adaptive chemical systems.

8. Contents

8.1. Course	**Teaching and learning methods**	**Remarks[3]**
8.1.1. General concepts in stereochemistry	Lecture, explanation, conversation description and problematization	Each subject is planned for 2h activity
8.1.2. Symmetry operations, symmetry groups	Lecture, explanation, conversation description and problematization	
8.1.3. Enantiomerism: optical activity, configuration descriptors	Lecture, explanation, conversation description and problematization	
8.1.4. Chirality: central, axial, planar, helicoidal and supramolecular. Prochirality.	Lecture, explanation, conversation description and problematization	
8.1.5. Diastereoisomers. Generalities. Configurational diastereoisomers; experimental methods for the determination of the configurations.	Lecture, explanation, conversation description and problematization	
8.1.6. Conformational analysis. Torsions in cyclic and acyclic compounds	Lecture, explanation, conversation description and problematization	
8.1.7. Supramolecular chemistry: generalities	Lecture, explanation, conversation description and problematization	
8.1.8. Non-covalent interactions (contacts)	Lecture, explanation, conversation description and problematization	
8.1.9. General methods for the access to macrocycles and mechanically interlocked molecules	Lecture, explanation, conversation description and problematization	
8.1.10. Properties of macrocycles and mechanically interlocked molecules	Lecture, explanation, conversation description and problematization	
8.1.11. Self-assembled supramolecular architectures	Lecture, explanation, conversation description and problematization	
8.1.12. Adaptative (covalent dynamic) chemistry	Lecture, explanation, conversation description and problematization	

Bibliography

1. S. Mager, I. Grosu, L. David, *Stereochimia Compușilor Organici*, Ed. Dacia, 2006
2. E. L. Eliel, S. Wilen, *Sterochemistry of Organic Compounds*, WILEY, 1994.
3. P. Y. Bruice, *Organic Chemistry*, Prentice Hall, 1998.
4. J. March, B. Smith, *Advanced Organic Chemistry*, Wiley, 2006.
5. Steed J. W., Atwood J. L. *Supramolecular Chemistry*, Wiley, New York, (2000).
6. Vögtle, F.; Stoddart, J. F. and Shibasaki, M (editors), *Stimulating Concepts in Chemistry*, Wiley-VCH, Weinheim, Germany (2000).
7 Diederich, F.; Stang, P. G. and Tykwinski, R. R. (editors), *Modern Supramolecular Chemistry-Strategies for Macrocycle Synthesis*, Wiley-VCH, Weinheim, Germany (2008)

8.2. Seminar/ laboratory	**Teaching and learning methods**	**Remarks**
8.2.1. Symmetry operations, symmetry groups. Enantiomerism: optical activity, configuration descriptors	explanation, conversation description and problematization	1h
8.2.2-3. Chirality: central, axial, planar, helicoidal and supramolecular. Prochirality	explanation, conversation description and problematization	2h

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

8.2.4. NMR applications in conformational analysis of acyclic, cycloalkanes and aliphatic heterocycles..	explanation, conversation description and problematization	1h
8.2.5-6. Geometric isomers. Stereochemistry of compounds with several stereogenic units.	explanation, conversation description and problematization	2h
8.2.7-8 Problems connected to macrocycles, cryptands and cyclophanes	explanation, conversation description and problematization	2h
8.2.9-10 Problems connected to host-guest supramolecular entities	explanation, conversation description and problematization	2h
8.2.11-12 Problems connected to self-assembled supramolecular architectures	explanation, conversation description and problematization	2h

Bibliography

Cãta, L.; Stroia, I.; Nicolay, C.; Hădade, N. D.; Terec, A.; Barboiu, M.; Grosu, I.,
"ExBoxes" with fluorene and carbazole units. Synthesis, structure determina-tion and formation of Host-Guest complexes. Synthesis-Stuttgart, **2025**, 57, 3579-3586
Cucuiet, T. A.; Anghel, C. C.; Pop, A.; Moisa, M. E.; Gautier, A.; Traikia, M.; Grosu, I.; Hădade, N. D.,
Efficient Synthesis of Conformationally Constrained 5,5′-Bi-1,2,3-Triazole-Based Bis-Macrocycles Synthesis-Stuttgart, **2025**, 57, 3462-3468
Anghel, C. C.; Cucuiet, T. A. ; Hădade, N. D.; Grosu, I. *Active-metal template clipping synthesis of novel [2]rotaxanes, Beil. J. Org. Chem.* **2023***, 19,* 1776-1784
Stroia, I.; Moisă, M. E.; Pop, A.; Legrand, B.; Hanganu, A.; Hădade, N. D.; Grosu, I.
Planar Chiral p,p'-Terphenyl-based Cyclophanes with Remarkable Enantiomers Stability: Synthesis, Theoretical Investigations and Complexation Studies; J. Org. Chem., **2023**, *88 (22)*, 15647−15657
Pop, L.; Grosu, I. G.; Miclăuș, M.; Hădade, N. D.; Pop, A.; Bende, A.; Terec, A.; Barboiu, M.; Grosu, I.
Halogen-Bonded Organic Frameworks of Perfluoroiodo- and Perfluorodiiodobenzene with 2,2′,7,7′-Tetrapyridyl-9,9′-spirobifluorene, *Cryst. Growth Des.,* **2021***, 21*, 1045-1054
Grosu, I. G.; Pop, L.; Miclăuș, M.; Hădade, N. D.; Terec, A.; Bende, A.; Socaci, C.; Bărboiu, M.; Grosu, I.
Halogen Bonds (N---I) at Work: Supramolecular Catemeric Architectures of 2,7-Dipyridylfluorene with ortho-, meta-, or para Diiodotetrafluorobenzene Isomers, Cryst. Growth Des., **2020***, 20*, 3429-3441
Lar, C.; Moisă, M.E.; Bogdan, E.; Terec, A.; Hădade, N. D.; Grosu, I.; David, L.; Paizs, C.; Grosu, I.G
"Geländer" macrocycles: Synthesis, chirality and racemisation barriers, Tetrahedron Lett., **2019**, *60*, 335-340
Diac, A., Matache, M., Grosu, I., Hădade, N.D., *Naphthalenediimide – A Unique Motif in Macrocyclic and Interlocked Supramolecular Structures, Adv. Synth. Catal.*, 2018, 360, 817-845
Rednic, M. I.; Varga, R. A.; Bende, A.; Grosu, I. G.; Miclăuș, M.; Hădade, N. D.; Terec, A.; Bogdan, E.; Grosu, I., *Supramolecular anion recognition by β-HCH, Chem. Commun.*, **2016**, *52*, 12322-12325

Last five years collections of journals Angew. Chem. Int. Ed.; Chem. Eur. J.; Eur. J. Org. Chem; Chem. Commun.; Chem. Sci.; Dalton Trans.; Org. Lett.; Organometallics; Inorg. Chem. and J. Org. Chem.

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	Th quality of the answers, the understanding of the problems	oral exam	60%
	The support given to the proposed solutions and their originality		
9.5. Seminar/ laboratory	Seminar activity	Papers presentations	40%
9.6 Minimum standard for passing			
5 (five)			

[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.

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

	○	Sustainable Development Generic Label

								
○	○	○	X	○	○	○	○	○
								No label applies
○	○	○	○	○	○	○	○	○

Date of entry:
26.01.2026

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



[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."*