UNIVERSITY of MISKOLC
Faculty of Materials andChemical Engineering

Antal Kerpely Doctoral School of Materials Science & Technology

Synthetic chemistry in industrial applications

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COURSE DESCRIPTION

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Synthetic chemistry in industrial applications

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Lecturer

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Recommendation

The lecture is offered for all students of the Kerpely Doctral School, especially in the field of chemistry.

Language

English

Scope

The aim of the course is to provide students with advanced, theoretically grounded, and reaction-focused knowledge in organic chemistry. Students will gain deeper insight into the interrelationships between reaction mechanisms, electronic effects, stereochemical factors, and synthetic methodologies. The course also aims to equip students with the ability to independently interpret complex reaction pathways and to design synthetic strategies.

Methodology

In case of a larger number of students, the course material is delivered through lectures and case study-based practical sessions. For small groups (1–2 students), the learning process is personalized: students receive the material in three thematic blocks, each accompanied by recommended literature and control questions. During consultation sessions, students' answers are evaluated orally, emerging questions are discussed, and the key concepts and examples of organic chemistry are reviewed in depth.

Learning outcomes

By the end of the course, students will be able to:

1. Analyze and rationalize complex organic reaction mechanisms using electron-pushing formalism.
2. Evaluate the effects of electronic, steric, and stereoelectronic factors on reactivity and selectivity.
3. Apply advanced synthetic methodologies, including C–C and C–X bond-forming reactions, to design multistep syntheses.
4. Utilize retrosynthetic analysis for the strategic disconnection of target molecules.
5. Interpret and predict the outcomes of pericyclic, radical, organometallic, and asymmetric reactions.
6. Integrate mechanistic understanding into the planning and optimization of synthetic routes for complex molecules.

Topics

1. Advanced Reaction Mechanisms and Theoretical Foundations

This block focuses on a deeper mechanistic understanding of organic reactions, including electron transfer processes, intermediates, and catalytic cycles.

- Electronic effects: inductive, resonance, hyperconjugation
- Mechanisms of nucleophilic and electrophilic reactions
- Characterization of carbocationic, carbanionic, and radical intermediates
- Pericyclic reactions: Diels–Alder, electrophilic cyclizations
- Basics of catalysis: acid–base, organometallic, and organocatalysis

2. Functional Group Transformations and Retrosynthetic Analysis

The goal of this block is to enable students to deconstruct complex molecules and design syntheses using retrosynthetic logic.

- Oxidation and reduction methods (e.g., Swern, PCC, $NaBH_4$, $LiAlH_4$, catalytic hydrogenation)
- C–C bond-forming strategies: Grignard, organolithium reagents, enolate chemistry
- Aldol reactions, Claisen condensation, Michael addition
- Stereoselective reactions and asymmetric synthesis
- Retrosynthetic strategies and reagent selection

3. Modern Synthetic Methods and Specialized Reaction Types

This block introduces modern and specialized synthetic tools and techniques, including organometallic catalysis, photochemistry, and ring-forming strategies.

- Organometallic cross-couplings: Suzuki, Heck, Sonogashira, Buchwald–Hartwig
- Modern carbocation and carbanion chemistry
- Photoredox and electrochemical methods
- Heterocycle synthesis and ring construction strategies
- Case studies from the synthesis of complex natural products or drug molecules

Control Questions

1. What is the difference between the SN1 and SN2 mechanisms?
2. List at least three types of pericyclic reactions.
3. How do the reactivities of an enol and an enolate differ?
4. Why are protecting groups important in synthetic organic chemistry?
5. How does the acidity of α-protons in carbonyl compounds depend on the nature of neighboring groups?
6. What is the role of palladium catalysts in cross-coupling reactions?
7. What is stereoselectivity and how does it differ from enantioselectivity?
8. How does retrosynthetic planning work in organic synthesis?
9. What is the essence of the Claisen condensation, and what conditions are required?
10. What types of intermediates are typical in radical reaction mechanisms?

References

Hungarian-language literature:

- Hudlicky – Hruby – Simig: *Szerves Kémia II.* textbook. Medicina, Budapest
- Zoltán Pápa (ed.): *Haladó szerves kémia példatár.* ELTE, in manuscript format

English-language literature:

- Clayden, Greeves, Warren, Wothers: *Organic Chemistry.* Oxford University Press
- Carey – Sundberg: *Advanced Organic Chemistry, Parts A and B.* Springer
- Michael B. Smith: *March's Advanced Organic Chemistry.* Wiley

Exam

Oral exam after correctly answering some basic questions.

Complex exam topics and sample questions

1. Explain the SN1, SN2, E1, and E2 reaction mechanisms and their competition using a representative example.
2. Describe the MO-based interpretation of pericyclic reactions (Woodward–Hoffmann rules).
3. Present the principles of retrosynthetic analysis using a complex organic molecule as an example.
4. Analyze an asymmetric reaction (e.g., Sharpless oxidation, CBS reduction) and explain how enantioselectivity is achieved.
5. Compare the Grignard reaction with enolate-based C–C bond-forming reactions in terms of advantages and limitations.
6. Explain the mechanism of the Suzuki cross-coupling reaction and its importance in synthetic planning.
7. What factors should be considered when selecting protecting groups in the synthesis of multifunctional molecules?
8. Present the key retrosynthetic steps in the total synthesis of a natural product or drug molecule.
9. Discuss the role of redox reactions in organic synthesis (e.g., Swern oxidation, Dess–Martin periodinane, catalytic reductions).
10. What is the significance of photochemical and electrochemical methods in modern organic synthesis?