

Universidade Federal do Rio Grande do Sul Instituto de Química

Graduate Program in Chemistry (Grade 7/CAPES)

Av. Bento Gonçalves, 9500 – Bairro Agronomia Porto Alegre, RS – Brazil - ZIP 91501970

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COURSE SYLLABUS

1. Identification

Code and title: QUP 302 - Advanced Organic Chemistry

Professor: Fabiano Severo Rodembusch, Diogo Seibert Lüdtke and Angélica Venturini Moro

Level: Master and Doctorate

Credit hours: 3

Revised: August 2021

2. Summary

Organic Physical chemistry applied to elucidate mechanisms of organic reactions; conformational effects and chemical reactivity in cyclic and acyclic systems

3. Objective

Discuss concepts for the elucidation of reaction mechanisms and advanced models in view of understanding the structures, properties and reactivity of organic compounds

4. Contents

- 4.1 Kinetics of simple and complex reactions and chemical equilibrium. Physical meaning of activation parameters. Steady state approximation for organic reactions. Hammond's Principle. Curtin-Hammett's principle. Determining step of reaction and composition of the activated complex. Diagrams by More O'Ferral. Catalytic effects specific and general acidic and basic catalysis. Nucleophile catalysis. Molecular isotopic effect. Primary and secondary isotopic kinetic effect of deuterium. Isotopic kinetic effect on the solvent. Solvation and solvent effect on chemical reactions.
- 4.2 Conformational effects and chemical reactivity of organic compounds steric, electronic and stereo-electronic effects in acyclic systems and cyclic systems application of the concepts developed in item 4.1 in aliphatic nucleophilic substitution reactions, electrophilic addition, beta eliminations, addition of nucleophiles and hydrolysis of carbonyl derivatives.
- 4.3 Enolization processes, Ireland model, carbonyl group addition models and Zimmerman-Traxler transition states in carbonyl compounds

5. Assessment

Lectures, exercises lists, seminars and examinations. The student who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:

A: grade equal to or above 9.0

B: grade equal to or above 7.5 and below 9.0

C: grade equal to or above 5.0 and below 7.5

D: grade below 5

FF: lack of frequency

6. Methodology



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Lectures, exercises lists, seminars and examinations.

7. Bibliography

- J. March, Advanced Organic Chemistry. Reactions, Mechanism and Structure, 4ª Ed. New York: John Wiley & Sons, 1992.
- F. Carey and R.J. Sundberg, Advanced Organic Chemistry. Part A and B. 3ª Ed. New York; Plenum Press, 1990.
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- T. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry. New York: Harper e Row Publ., 1987.
- J. Hine, Physical Organic Chemistry. McGraw-Hill Editor, 1962.
- I. Fleming, Frontier Orbitals and Organic Chemical Reactions, John Wiley & Sons, 1986.
- N. Issacs, Physical Organic Chemistry, 2nd edition, Longman Scientific & Technical, 1995.
- Eric V. Anslyn, Dennis A. Dougherty (Authors), Modern Physical Organic Chemistry, University Science; illustrated edition (July 15, 2005).