University of Gdańsk

Subject card

Subject name and code	Insights into reaction mechanisms and kinetics via quantum chemistry methods, PG_00119776						
Field of study	Chemistry						
Date of commencement of studies	October 2025		Academic year of realisation of subject	2026/2027			
Education level	Master's studies		Subject group	Optional subject group			
Mode of study	full-time studies		Mode of delivery	at the university			
Year of study	2		Language of instruction	English			
Semester of study	3		ECTS credits	2.0			
Learning profile	academic		Assessment form	credit			
Conducting unit	Laboratory of Quantum Chemistry -> Department of Theoretical Chemistry -> Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Iwona Anusiewicz				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	30.0	0.0	0.0	30
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan		Participation in consultation hours	Self-study	SUM	
	Number of study hours	30		5.0	15.0	50	
Subject objectives	Acquiring the knowledge of the fundamental terms related to the mechanisms of chemical reactions. Acquiring the ability to evaluate the activation barriers and thermodynamic barriers of chemical reactions. Acquiring the ability to use theoretical methods for prediction of the rate constants of chemical reactions.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_U04] Applies acquired knowledge of chemistry and related scientific disciplines.	Student has the ability of locating transition states on the reaction path,	[SU2] presentation/project/paper/ report
[CHEMMU2_W08] Demonstrates knowledge of theoretical computational and IT methods used to solve problems in chemistry.	Student defines and describes basic terms related to the mechanisms of chemical reactions, understands the role of activation barriers on the reaction rate constant,	[SW2] presentation/project/paper/ report
[CHEMMU2_U05] Presents the results of research in the form of an independently written paper containing a description and justification of the purpose of the work, adopted methodology, results and their significance in comparison to other similar research.	Student has the ability of calculating the reaction rate constant and providing the overall reaction picture	[SU2] presentation/project/paper/ report
[CHEMMU2_W07] Selects experimental and theoretical techniques to the extent necessary to understand the description and modelling of medium complexity chemical processes.	Student knows how to choose the proper theoretical methods	[SW2] presentation/project/paper/ report
[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	Student has the ability of estimating the heights of activation barriers and thermodynamic barriers	[SU2] presentation/project/paper/ report
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Student knows how to perform the study of a given reaction mechanism.	[SW2] presentation/project/paper/ report
[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Student develops the skills of accurate and logical thinking and inference. Learns the principles of working safely, responsibly, and efficiently. Develops the ability to work in a team.	[SK2] presentation/project/paper/ report

Subject contents

The course covers the explanation of fundamental terms related to the mechanisms of chemical reactions, including the formulas required to calculate the reaction rate constant. The students will be taught how to obtain an overall picture of the reaction mechanism, distinguish between concerted and stepwise mechanisms, finding initial complexes of reagents, locating transition states (saddle points) and intermediate products, estimating the heights of kinetic (activation) barriers, evaluating the heights of thermodynamic barriers, and calculating the rate constants. These abilities will be taught by studying the real examples of various reaction mechanisms with the use of computational quantum chemistry tools.

Prerequisites and co-requisites

basic knowledge in chemistry

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Assessment criteria in accordance with the University of Gdańsk Study Regulations Laboratory classes: grades based on the quality of the solutions of the assigned exercises	51.0%	100.0%

Recommended reading

Basic literature	Energetic Principles of Chemical Reactions, J. Simons, Jones and Bartlett Publishers, Inc., 1983.An Introduction to Theoretical Chemistry, J. Simons, Cambridge University Press, 2003
Supplementary literature	Geometrical Derivative of Energy Surfaces and Molecular Properties, P. Jorgensen, J. Simons, D. Reidel Publishing Company, 1985
eResources addresses	

Example issues/ example questions/ tasks being completed

Calculate the reaction rate constant for the CH_3CN-->CH_3NC transformation in the gas phase and in water solvent.

Work placement

Not applicable

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