

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 2024	Academic year of realisation of subject			2025/2026		
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					
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	<p>Acquiring the knowledge of the fundamental terms related to the mechanisms of chemical reactions.</p> <p>Acquiring the ability to evaluate the activation barriers and thermodynamic barriers of chemical reactions.</p> <p>Acquiring the ability to use theoretical methods for prediction of the rate constants of chemical reactions.</p>						

Learning outcomes	Course outcome	Subject outcome	Method of verification
	[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
	[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_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_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_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_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_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	
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	Adresy na platformie eNauczanie:	
Example issues/example questions/tasks being completed	Calculate the reaction rate constant for the $\text{CH}_3\text{CN} \rightarrow \text{CH}_3\text{NC}$ transformation in the gas phase and in water solvent.		
Work placement	Not applicable		

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