

(Table 5.2) Course unit description

Study program: Chemistry Ph.D			
Type and level of studies: Doctoral academic studies			
Course unit: Molecular Modeling in Organic Chemistry			
Teacher in charge: Slavko D. Radenković			
Language of instruction: English			
ECTS: 10			
Prerequisites: Enrolled semester			
Semester: Summer semester			
Course unit objective The aim of the course is to extend students' knowledge and skills in molecular modeling, which will facilitate their study and research in chemistry, using quantum-mechanical methods.			
Learning outcomes of Course unit Students will acquire knowledge in the field of modeling chemical interaction using different computational methods, and the skill in using the Gaussian program package.			
Course unit contents <i>Theoretical classes:</i> Energy levels in atoms and molecules. Relationship between molecular energy levels and thermodynamic quantities. Calculation of vibrational frequencies in molecules; modeling of IR spectra. Hierarchy of quantum chemical methods. Post-Hartree–Fock methods. Configuration interaction (CI) method. Møller–Plesset (MP) methods. Multiconfigurational self-consistent field (MCSCF) theory. Density functional theory. Modeling of magnetic properties of molecules. <i>Practical classes:</i> Simulation of different types of molecular spectra: UV-Vis, IR, NMR.			
Literature 1. Frank Jensen, <i>Introduction to Computational Chemistry</i> , John Wiley & Sons, Chichester, 2007. 2. James B. Foresman, Aileen Frisch: <i>Exploring Chemistry with Electronic Structure Methods</i> , third edition, Gaussian, Inc. Wallingford, CU USA, 2015. 3. Gaussian Inc., Pittsburgh PA, USA: Gaussian Help Table of Contents.			
Number of active teaching hours 5			Other classes:
Lectures: 5	Practice:	Other forms of classes: Independent work:	
Teaching methods Problem-oriented teaching, practical training, seminar works, assignments.			
Examination methods (maximum 100 points)			
Exam prerequisites	No. of points	Final exam	No. of points
Practical classes		Written examination	30
Tests		Oral examination	25
Homework		Other	
Seminars	15		
Project	30		
Grading system			
Grade	No. of points	Description	
10	>= 91	Excellent	
9	81-90	Exceptionally good	

8	71-80	Very good
7	61-70	Good
6	51-60	Passing
5	<=50	Failing