

Study program: Chemistry			
Type and level of studies: Master academic studies in Chemistry			
Course unit: Molecular modeling 2			
Teacher in charge: Svetlana Marković			
Language of instruction: English			
ECTS: 6			
Prerequisites: Passed courses Molecular modeling 1 or Molecular modeling in teaching chemistry			
Semester: Winter semester			
Course unit objective			
The course aims to expand students' knowledge and skills acquired in the courses Molecular Modeling 1 or Molecular modeling in teaching chemistry, which will facilitate the study and research of chemistry, using molecular-mechanical and quantum-mechanical methods.			
Learning outcomes of Course unit			
Students will gain knowledge in the field of modeling of chemical interactions using various computational methods, and skills in using the Gaussian program package.			
Course unit contents			
<i>Theoretical classes</i>			
Post-Hartree-Fock methods: semiempirical methods, configuration interaction, Møller-Plesset methods, multiconfigurational self-consistent field theory, density functional theory; vibrational frequencies and thermodynamic quantities, thermochemical data output from Gaussian; reaction energies; equilibrium conformations.			
<i>Practical classes</i>			
Learning how to use the software package Gaussian. Calculating translational, electronic, rotational and vibrational contributions to the entropy, heat capacity and thermal correction. Scaling the thermochemical quantities. Singlet - triplet separation, complete active space method. Absolute acidity and basicity. Isodesmic reactions: relative acidity and basicity, determination of the heat of formation by using the bond separation reactions. Calculation of the barriers for rotation around single bond and pyramidal inversion. Searching the conformational space. Determination of reactive conformers.			
The student should, in consultation with the professor, do a project. This means that computational methods should be applied to the selected chemical problem, and the obtained results be presented in written and oral forms.			
Literature			
Gaussian Inc., Pittsburgh PA, USA: Gaussian Help Table of Contents. Electronic version of this textbook can be downloaded from the Internet.			
Number of active teaching hours			Other classes
Lectures: 2	Practice: 2	Other forms of classes: mentoring system	Independent work: 0
Teaching methods			
Problem-oriented teaching, practical training, project, homework assignments.			
Examination methods (maximum 100 points)			
Exam prerequisites	No. of points:	Final exam	No. of points:
Student's activity during lectures	Can make influence	oral examination	30
practical classes/tests	10	written examination	30
Seminars/homework	Makes influence	
Project	30		
Other			
Grading system			
Grade	No. of points	Description	
10	> 90	Excellent	
9	80 ≥ 90	Exceptionally good	
8	70 ≥ 80	Very good	
7	60 ≥ 70	Good	

6	$50 \geq 60$	Passing
5	< 60	Failing

(Table 5.2) Course unit description