(Table 5.2) Course unit description

Study program: Chemistry				
Type and level of studies: Doctoral academic studies in Chemistry				
Course unit: Molecular modeling in Organic chemistry				
Teacher in charge: Svetlana Marković				
Language of instruction: English				
ECTS: 10				
Prerequisites: Passed courses Molecular modeling 1 or Molecular modeling in teaching chemistry and Molecular modeling 2				
Semester: Summer semester				
Course unit objective Students will be introduced to the simulation of various chemical spectra using the software for molecular modeling, and the application of solvation models to the investigation of the reaction mechanisms. They will acquire skills in using the Gaussian program package and independence in modeling of different chemical phenomena in the field of organic chemistry, with the possibility of applying to the specific chemical problems that are of interest to the student concerned.				
Learning outcomes of Course unit Students will complement understanding of organic chemistry in a way that solving chemical problems will be based on a set of molecular models, which will considered and manipulated with by using computer programs. This combination of problems and molecular models will improve the understanding of molecular structure and the relationship between molecular structure and other characteristics.				
Course unit contents *Theoretical classes* Optimized geometry and experimental structure, simulation of the NMR, IR and UV/Vis spectra, salvation models, mechanisms of organic reactions.				
Literature 1**.** J. B. Foresman, Æ. Frisch: *Exploring chemistry with electronic structure methods*, Gaussian Inc. (1993) Pittsburgh. 2. Scientific papers				
Number of active teaching hours				**Other classes**
Lectures: 5	Practice: 0	Other forms of classes: mentoring system	Independent work: 0	
Teaching methods Lectures, consultations, projects				
Examination methods (maximum 100 points)				
Exam prerequisites	**No. of points:**	**Final exam**	**No. of points:**	
Student's activity during lectures	10	oral examination	30	
practical classes/tests		written examination	30	
Seminars/homework		.....		
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 ≥ 60	Passing
5	< 60	Failing