

**Table 5.2** Course description

Study program: Chemistry, Master's program			
Course title: Quantum chemistry			
Professor: Slavko Radenković			
Course type:			
ECTS credits: 5			
Prerequisites: BSc degree in Chemistry or related sciences			
<b>Course objectives</b>			
The aim of the course is to provide students with a fundamental understanding of the quantum chemical description of atoms and molecules.			
<b>Learning outcomes</b>			
Students who successfully pass this exam can use the obtained knowledge of quantum chemical principles and the necessary mathematical techniques in their experimental and theoretical studies of molecules and molecular phenomena.			
<b>Course topics</b>			
<i>Theoretical classes</i>			
Principles of wave mechanics; atomic orbitals; atomic orbitals in many-electron atoms.			
Mathematical foundations of quantum mechanics: vector space, operators, representations; postulates of quantum mechanics; angular momentum; perturbation and variational methods.			
Symmetry of molecules and orbitals; symmetry operations; group theory and its application in chemistry.			
Valence bond and molecular orbital theory; hydrogen molecule; self-consistent field (Hartree-Fock) theory; post Hatree-Fock methods.			
Nuclear Schrödinger equation; Born-Openheimer approximation; harmonic oscillator; vibrations in many-atom molecules; symmetry of vibrational modes; molecular rotation; selection rules			
<i>Practical classes</i>			
Practical classes should help students to better understand the subject presented in the theoretical classes.			
<b>Recommended literature</b>			
1. P.W. Atkins, <i>Molecular Quantum Mechanics</i> , Oxford Univerity Press, 1983.			
2. A. Szabo, N.S. Ostlund, <i>Modern Quantum Chemistry</i> , Macmillan Publishing Co., New York, 1882.			
<b>Number of classes of active teaching</b>			Other classes
Lectures: 2	Practicals: 2	Other forms of teaching: Consultations	
<b>Teaching methods</b>			
Problem-oriented teaching, practical training, seminar works, assignments.			
<b>Knowledge assessment (maximum score 100)</b>			
<b>Pre-exam obligations</b>	<b>points</b>	<b>Exam</b>	<b>points</b>
activity during the course	5	written	20
practical classes	5	oral	30
colloquium(s)	30		
Seminar(s)	10		