(Table 5.2) Course unit description

<table>
<tr><td colspan="5">Study program: Chemistry</td></tr>
<tr><td colspan="5">Type and level of studies: Master academic studies</td></tr>
<tr><td colspan="5">Course unit: Molecular Modeling</td></tr>
<tr><td colspan="5">Teacher in charge: Slavko D. Radenković</td></tr>
<tr><td colspan="5">Language of instruction: English</td></tr>
<tr><td colspan="5">ECTS: 5</td></tr>
<tr><td colspan="5">Prerequisites: Enrolled semester</td></tr>
<tr><td colspan="5">Semester: Summer semester</td></tr>
<tr><td colspan="5">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 molecular-mechanical and quantum-mechanical methods.</td></tr>
<tr><td colspan="5">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.</td></tr>
<tr><td colspan="5">Course unit contents
Theoretical classes:
Energy levels in atoms and molecules. Relationship between molecular energy levels and thermodynamic quantities. Calculation of vibrational frequencies in molecules; modeling of IR spectra. Calculation of thermodynamic quantities. Modeling of equilibrium conformations of molecules. Modeling reaction changes of thermodynamic quantities. Hierarchy of quantum chemical methods. Post-Hartree–Fock methods. Semi-empirical methods. Configuration interaction (CI) method. Møller–Plesset (MP) methods. Multiconfigurational self-consistent field (MCSCF) theory. Density functional theory. Population analysis. Modeling of magnetic properties of molecules.
Practical classes:
Calculation of translational, electronic, rotational, and vibrational contributions to the entropy, thermal capacity at constant volume, and thermal correction. Scaling factors for thermochemical quantities. Singlet-triplet energy gap, CASSCF method. Absolute acidity and basicity. Isodesmic reactions: relative acidity and basicity, application of bond separation reactions to determination of the heat of formation. Calculation of the barriers to rotation and pyramidal inversion. Searching the conformational space. Determination of reactive conformer. Each student should prepare one seminar work. This implies that computational methods will be applied on a selected chemical problem. Consultations with the professor are planned. The results obtained need to be presented in written and oral forms.</td></tr>
<tr><td colspan="5">Literature
1. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons, Chichester, 2007.
2. James B. Foresman, Æleen Frisch: Exploring Chemistry with Electronic Structure Methods, third edition, Gaussian, Inc. Wallingford, CU USA, 2015.
3. Gaussian Inc., Pittsburgh PA, USA: Gaussian Help Table of Contents.</td></tr>
<tr><td colspan="4">Number of active teaching hours</td><td rowspan="2">Other classes:</td></tr>
<tr><td>Lectures:
2</td><td>Practice:
2</td><td>Other forms of classes:</td><td>Independent work:</td></tr>
<tr><td colspan="5">Teaching methods
Problem-oriented teaching, practical training, seminar works, assignments.</td></tr>
</table>

Examination methods (maximum 100 points)			
Exam prerequisites	**No. of points**	**Final exam**	**No. of points**
Practical classes	10	Written examination	25
Tests	30	Oral examination	20
Homework	5	Other	
Seminars	10		
Project			

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