(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’s program</td></tr>
<tr><td colspan="5">Course unit: Molecular modeling 2</td></tr>
<tr><td colspan="5">Teacher in charge: Svetlana D. Marković</td></tr>
<tr><td colspan="5">Language of instruction: English</td></tr>
<tr><td colspan="5">ECTS: 6</td></tr>
<tr><td colspan="5">Prerequisites: Molecular modeling 1 or analogous course Semester: summer</td></tr>
<tr><td colspan="5">Course unit objective
The aim of the course is to extend students' knowledge and skills acquired at Molecular modeling 1 (or analogous course), which will facilitate their study and research of 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
Post-Hartree-Fock methods: semiempirical methods, configurational interaction, Møller-Plesset methods, multiconfigurational self-consistent field theory, density functional theory; vibrational frequencies and thermodynamic quantities, Gaussian thermochemistry output; reaction energies; equilibrium conformations.
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, complete active space method. Absolute acidity and basicity. Isodesmic reactions: relative acidity and basicity, application of bond separation reactions to determination of the heat of formation. Searching the conformational space. Construction and calculation of all cyclohexane conformers.
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 the written and oral forms.</td></tr>
<tr><td colspan="5">Literature
1. James B. Foresman, Æleen Frisch: Exploring Chemistry with Electronic Structure Methods, third edition, ISBN 978-1-935522-03-4, Gaussian, Inc. Wallingford, CU USA (2015).
2. Gaussian Inc., Pittsburgh PA, USA: Gaussian Help Table of Contents.
3. Scientific papers.</td></tr>
<tr><td colspan="4">Number of classes of active teaching hours</td><td>Other classes</td></tr>
<tr><td>Lectures:
2</td><td>Practice:
2</td><td>Other forms of classes:
Consultations</td><td colspan="2">Independent work:</td></tr>
<tr><td colspan="5">Teaching methods
Problem-oriented teaching, practical training, seminar works, assignments.</td></tr>
<tr><td colspan="5">Examination methods (maximum 100 points)</td></tr>
<tr><td>Exam prerequisites</td><td>No. of points</td><td>Final exam</td><td colspan="2">No. of points</td></tr>
<tr><td>Activity during the course</td><td>can influence the mark</td><td>Written examination</td><td colspan="2">30</td></tr>
<tr><td>Practical classes</td><td>10</td><td>Oral examination</td><td colspan="2">30</td></tr>
<tr><td>Seminar(s)</td><td>30</td><td></td><td colspan="2"></td></tr>
<tr><td colspan="5">Grading system</td></tr>
<tr><td colspan="2">Grade</td><td colspan="2">No. of points</td><td>Description</td></tr>
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10	> 90	Excellent
9	80 ≥ 90	Exceptionally good
8	70 ≥ 80	Very good
7	60 ≥ 70	Good
6	50 ≥ 60	Passing
5	< 60	Failing