Table 5.2 Course description

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<tr><td colspan="5">Study program: Chemistry, Master’s program</td></tr>
<tr><td colspan="5">Course title: Molecular modeling 2</td></tr>
<tr><td colspan="5">Professor: Slavko Radenković</td></tr>
<tr><td colspan="5">Course type: compulsory</td></tr>
<tr><td colspan="5">ECTS credits: 5</td></tr>
<tr><td colspan="5">Prerequisites: Molecular modeling 1 or analogous course</td></tr>
<tr><td colspan="5">Course objectives
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
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 topics
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. 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 the written and oral forms.</td></tr>
<tr><td colspan="5">Recommended 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</td><td>Other classes</td></tr>
<tr><td>Lectures:
2</td><td>Practicals:
2</td><td>Other forms of teaching:
Consultations</td><td colspan="2">Research work: 0</td></tr>
<tr><td colspan="5">Teaching methods
Problem-oriented teaching, practical training, seminar works, assignments.</td></tr>
<tr><td colspan="5">Knowledge assessment (maximum score 100)</td></tr>
<tr><td>Pre-exam obligations</td><td>points</td><td>Exam</td><td colspan="2">points</td></tr>
<tr><td>activity during the course</td><td>can influence the mark</td><td>written</td><td colspan="2">30</td></tr>
<tr><td>practical classes</td><td>10</td><td>oral</td><td colspan="2">30</td></tr>
<tr><td>colloquium(s)</td><td></td><td></td><td colspan="2"></td></tr>
<tr><td>seminar(s)</td><td>30</td><td></td><td colspan="2"></td></tr>
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