



<b>Course ID:</b> HFHI03	<b>Course name: INTRODUCTION TO CHEMICAL GRAPH THEORY</b>		
<b>Cycle: SECOND</b>	<b>Year: FIRST</b>	<b>Semester: I</b>	<b>ECTS credits: 4</b>
<b>Course status: ELECTIVE</b>	<b>Total course hours:</b> Lectures: 45 Auditory: 15		
<b>Teaching participants:</b>	<b>Teachers and associates with expertise in the field to which the subject belongs</b>		
<b>Prerequisite for enrollment:</b>	-		
<b>Course aims:</b>	Acquiring basic knowledge of the concepts and most important applications of graph theory in chemistry.		
<b>Thematic course units:</b>	<ol style="list-style-type: none"><li>1. Graphs and molecular graphs.</li><li>2. Chemistry major types of graphs.</li><li>3. Chemistry major concepts of graph theory.</li><li>4. Graphs and matrix of graphs. Graph spectra.</li><li>5. The trees and chemical trees.</li><li>6. Basic characteristics of trees. Extremal trees.</li><li>7. Benzenoid systems.</li><li>8. Basic structural characteristics of benzenoid systems.</li><li>9. Mathematical aspects of the Clar theory.</li><li>10. Counting graphs and isomers. The theory of counting.</li><li>11. Molecular and structural descriptors.</li><li>12. Application of structural descriptors - QSPR and QSAR. Examples from practice.</li><li>13. Graph theory and molecular orbitals.</li><li>14. Connection HMO theory and spectral graph theory.</li><li>15. The total <math>\pi</math>-electron energy.</li></ol>		
<b>Learning outcomes:</b>	<b>Knowledge:</b> Acquired basic knowledge of the concepts and applications of graph theory in chemistry. <b>Skills:</b> Drawing conclusions about phenomena related to the structure and properties of molecules by analyzing computational data. <b>Competences:</b> Application of acquired knowledge and skills in professional and specialist subjects in various fields of chemistry.		
<b>Teaching methodology:</b>	Lectures (oral presentation and interactive classes) Auditory exercises		

<b>Assessment methods and grading system<sup>1</sup>:</b>	<b>Grading criteria</b>		
	Criteria	Maximal score	Required score
	1. Class attendance	5	3
	2. Class activities	15	8
	3. Midterms	40	22
	4. Final exam	40	22
	Total	100	55
	<b>Scores and grading</b>		
	Score	Grade (BiH)	Grade (ECTS)
	< 55	5	F, FX
	55–64	6	E
	65–74	7	D
	75–84	8	C
85–94	9	B	
95–100	10	A	
<b>Literature<sup>2</sup>:</b>	<p><b>Mandatory literature:</b> /</p> <p><b>Supplementary literature:</b></p> <ol style="list-style-type: none"> <li>Ivan Gutman, <i>Uvod u hemijsku teoriju grafova</i>, Prirodno-matematički fakultet, Kragujevac, 2003.</li> <li>Milan Randić, Aromaticity of Polycyclic Conjugated Hydrocarbons, <i>Chemical Reviews</i>, 103, 3449-3605, 2003.</li> <li>Ivan Gutman, Sven J. Cyvin, <i>Introduction to the Theory of Benzenoid Hydrocarbons</i>, Springer-Verlag, Berlin, 1989.</li> </ol>		

<sup>1</sup>The grading structure for each subject is determined by the Council of the organizational unit before the beginning of the academic year in which the subject is taught as per Article 64, paragraph 6 of the Law on Higher Education of Sarajevo Canton

<sup>2</sup>The Senate of the higher education institution, as an institution, or the Council of the organizational unit of the higher education institution, as a public institution, determines by a special decision, which is published on its website before the beginning of the academic year obligatory, mandatory and recommended textbooks and manuals, as well as other recommended literature based on which exams are prepared and taken as per Article 56, paragraph 3 of the Law on Higher Education of the Sarajevo Canton