Univerza v Mariboru

Fakulteta za naravoslovje in matematiko

| UČNI NAČRT PREDMETA / COURSE SYLLABUS | |
|---|---|
| **Predmet:** | **Matematika v kemiji** |
| **Course title:** | **Mathematics in chemistry** |

| Študijski program in stopnja<br>Study programme and level | Študijska smer<br>Study field | Letnik<br>Academic year | Semester<br>Semester |
|---|---|---|---|
| **Izobraževalna kemija, 1. stopnja** | | **2. ali 3.** | **zimski ali poletni** |
| **Educational Chemistry, 2nd degree** | | | |

Vrsta predmeta / Course type: **Izbirni/elective**

**Univerzitetna koda predmeta / University course code:**

| Predavanja<br>Lectures | Seminar<br>Seminar | Vaje<br>Tutorial | Lab. vaje<br>Laboratory work | Druge oblike študija | Samost. delo<br>Individ. work | ECTS |
|---|---|---|---|---|---|---|
| **20** | | **10** | | | **150** | **6** |

**Nosilec predmeta / Lecturer:** Petra Žigert Pleteršek

| **Jeziki / Languages:** | | |
|---|---|---|
| | **Predavanja / Lectures:** | **Slovenski/Slovenian** |
| | **Vaje / Tutorial:** | **Slovenski/Slovenian** |

**Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:**

Matematika, Organska kemija I

**Prerequisits:**

Mathematics, Organic chemistry I

**Vsebina:**

- **Matrični račun:**

matrike in računske opracije na matrikah, obratna matrika, računanje determinante matrike, reševanje sistemov linearnih enačb

- **Osnove teorije grafov:**

definicija grafa, izomorfni grafi, posebne vrste grafov, sosednostna matrika, matrika razdalj, spekter grafa.

**Content (Syllabus outline):**

- **Matrix calculation**

matrices and operations with matrices, inverse matrix, calculation of the determinant, methods of solving of sistems of linear equations.

- **Fundamentals of graph theory:**

definition of a graph, isomorphic graphs, special graphs, matchings, adjacency matrix, distance matrix, spectrum of a graph.

- **Molekulski grafi:**

matematični model ogljikovodikov, aciklični grafi, karakteristični polinom, benzenoidni grafi.

- **Topološki indeksi:**

vloga topoloških indeksov, Wienerjev indeks, Szegedški indeks, Randićev indeks, Hosojev indeks in Hosoyev polinom, hiper-Wienerjev indeks, osnove QSAR, QSPR.

- **Resonančne strukture:**

Kekulejeve strukture in metode za njihov izračun, Clarove strukture in Clarovo število, struktura resonančnih grafov, Fibonaccijeve kocke

- **Molecular graphs:**

mathematical model of hydrocarbons, acyclic graphs, characteristic polynomial, benzenoid graphs.

- **Topological indices:**

role of the topological inices, Wiener index, Szeged index, Randić index, Hosoya index and Hosoya polynomial, hyper-Wiener index, basic ideas of QSAR,QSPR.

- **Resonance structures:**

Kekule structures and the methods for their calculation, Clar structures and Clar number, structure of the resonance graphs, Fibonacci cubes.

**Temeljni literatura in viri / Readings:**

- Ivan Gutman, Sven J. Cyvin, Introduction to theory of benzenoid hydrocarbons, Berlin, Springer-Verlag, 1989,
- Ivan Gutman, Oskar R. Polansky, Mathematical concepts in organic chemistry, Berlin, Springer-Verlag, 1986,
- Sandi Klavžar, Petra Žigert, Izbrana poglavja uporabne matematike, Maribor, Pedagoška fakulteta, 2002.

**Cilji in kompetence:**

- študent naj pridobi in utrdi osnovna znanja matričnega računa in teorije grafov in jih zna aplicirati pri reševanju problemov s področja kemije,
- študent naj spozna matematični model strukture nekaterih ogljikovodikov in vlogo topoloških indeksov.

**Objectives and competences:**

- the student should gain and establish the basic mathematical knowledge about matrix calculation and graph theory and knows how to use it in solving chemical problems,
- the student is familiar with the mathematical model of structure of some hydrocarbons and the use of topological indices.

**Predvideni študijski rezultati:**

Znanje in razumevanje:

- študent pozna osnove teorije grafov in jih zna prenesti na matematično modeliranje strukture nekaterih ogljikovodikov,
- študent zna izračunati nekatere

**Intended learning outcomes:**

Knowledge and Understanding:

- the student is familiar with the basic concepts of graph theory and knows how to use them in the mathematical modeling of structure of some hydrocarbons,
- the student knows how to calculate

| | |
|---|---|
| topološke indekse ogljikovodikov,<br><br>- študent pozna resonačne grafe in zna poiskati število Kekulejevih struktur ter Clarovo število.<br><br>Prenesljive/ključne spretnosti in drugi atributi:<br><br>- matematično modeliranje v organski kemiji,<br><br>- interdisciplinarnost matematike in kemije. | some topological indices of hydrocarbons,<br><br>- the student is familiar with the resonance graphs and can find the number of Kekule structures and Clar number.<br><br>Transferable/Key Skills and other attributes:<br><br>- mathematical modeling in the organic chemistry,<br><br>- interdisciplinarity of mathematics and chemistry. |

| **Metode poučevanja in učenja:** | **Learning and teaching methods:** |
|---|---|
| - predavanja in seminarsko delo. | - lectures and a seminar work. |

| **Načini ocenjevanja:** | Delež (v %) / Weight (in %) | **Assessment:** |
|---|---|---|
| Način (pisni izpit, ustno izpraševanje, naloge, projekt) | | Type (examination, oral, coursework, project): |
| - seminarska naloga, | 20% | - a seminar work, |
| - ustni izpit. | 80% | - an oral exam. |

| **Materialni pogoji za izvedbo predmeta :** | **Material conditions for subject realization** |
|---|---|
| • računalnik in projektor | • a computer with the projector |

**Obveznosti študentov:** **Students' commitments:**

| *(pisni, ustni izpit, naloge, projekti)* | *(written, oral examination, coursework, projects):* |
|---|---|
| • seminarska naloga in prisotnost na predstavitah seminarskih nalog,<br><br>• ustni izpit. | • a seminar work and presence at the semianr work presentations,<br><br>• an oral exam. |

**Opomba:** **Navedene sestavine so obvezna sestavina učnega načrta predmeta kot ga določajo Merila za akreditacijo visokošolskih zavodov in študijskih programov v 7. členu (Ur. l. RS, št. 101/2004).**

**Reference nosilca / Lecturer's references:**

**1.** BALAKRISHNAN, Kannan, BREŠAR, Boštjan, CHANGAT, Manoj, KLAVŽAR, Sandi, VESEL, Aleksander, ŽIGERT PLETERŠEK, Petra. Equal opportunity networks, distance-balanced graphs, and Wiener game. *Discrete optimization*, ISSN 1572-5286, May 2014, vol. 12, str. 150-154, doi:

10.1016/j.disopt.2014.01.002. [COBISS.SI-ID 17782806]

**2.** ŽIGERT PLETERŠEK, Petra, BERLIČ, Martina. The structure of Lucas cubes and maximal resonant sets of cyclic fibonacenes. *MATCH Communications in Mathematical and in Computer Chemistry*, ISSN 0340-6253, 2013, vol. 69, no. 3, str. 707-720. [COBISS.SI-ID 16559894]

**3.** ŽIGERT PLETERŠEK, Petra, BERLIČ, Martina. Resonance graphs of armchair nanotubes cyclic polypyrenes and amalgams of Lucas cubes. *MATCH Communications in Mathematical and in Computer Chemistry*, ISSN 0340-6253, 2013, vol. 70, no. 2, str. 533-543. [COBISS.SI-ID 17253398]

**4.** TARANENKO, Andrej, ŽIGERT PLETERŠEK, Petra. Resonant sets of benzenoid graphs and hypercubes of their resonance graphs. *MATCH Communications in Mathematical and in Computer Chemistry*, ISSN 0340-6253, 2012, vol. 68, no. 1, str. 65-77. http://www.pmf.kg.ac.rs/match/content68n1.htm. [COBISS.SI-ID 16051990]

**5.** ŽIGERT PLETERŠEK, Petra, BERLIČ, Martina. Lucas cubes and resonance graphs of cyclic polyphenanthrenes. *MATCH Communications in Mathematical and in Computer Chemistry*, ISSN 0340-6253, 2012, vol. 68, no. 1, str. 79-90. http://www.pmf.kg.ac.rs/match/content68n1.htm. [COBISS.SI-ID 16050198]