|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| 1. Course title: Chemical Informatics | | | | | |
|  | | | | |
| 2. Code: | | 3. Type (lecture, practice etc.): lecture | | | |
|  | | | | |
| 4. Contact hours: 2 hoursper week | | 5. Number of credits (ECTS): 3 | | | |
|  | | | | |
| 6. Preliminary conditions (max. 3):  Physical Chemistry II. lect. | | | | | |
|  | | | | |
| 7. Announced:fall semester, spring semester, both | | | | | |
|  | | | | |
| 8. Limit for participants: - | | | | | |
|  | | | | |
| 10. Responsible teacher (faculty, institute and department):  Sándor Kunsági-Máté, PhD (Faculty of Science, Institute of Chemistry, Department of General and Physical Chemistry) | | | | | |
|  | | | | |
| 11. Teacher(s) and percentage: | | Dr. Beáta Lemli | | 100 % | |
|  | |  | |
|  | |  | |
|  | |  | |
|  | |  | |
|  | | | | |
| 12. Language:English | | | | | |
|  | | | | |
| 13. Course objectives and/or learning outcomes: Cognition of electronic sources necessary to earn chemical information and keeping it up to date with the aim that students are able to fast search of modern knowledge after finishing their studies. Based on the present computer and chemometrical knowledge applications are showed on chemical examples. | | | | | |
|  | | | | |
| 14. Course outline   1. Idea of information, description, types of information, tools getting information. Scientific communication. 2. Chemical informatics, computation sciences, statistics and molecular design. Different types of databases, ordered lists. 3. On-line databases on the internet, searching algorithm. Searching in the literature, chemical databases and its usage. 4. Computer nets and operation systems. Usage of supercomputers from terminals. 5. Vectorized computers and their optimal usage. Solvation of high calculations with extremely large CPU claim such as molecular modeling and geometry optimization. 6. Softwares for evaluation of experimental results. Usage of Excel. 7. Softwares for evaluation of experimental results. Usage of Origin. 8. Applications: calculation of chemical equilibrium, analtical and iterative methods. Determination of complex stability. Considering the parameters determining the stoichiometry. 9. Applications: Methods to determine reaction rates. Determining the chemical reaction order. 10. Kinetic box-models. 11. Overview on evaluation of experimental results according to the laboratory practice. 12. Overview on evaluation of experimental results according to the laboratory practice. 13. Overview on evaluation of experimental results according to the laboratory practice. | | | | | |
|  | | | | |
| 15. Mid-semester works  Attending lectures is highly recommended. | | | | | |
|  | | | | |
| 16. Course requirements and grading  Oral exam starts with a short test. Solving it the student proves that she/he could learn the basic definitions, equations, laws, and has the necessary problem solving expertise. After successful test the student draws two question leaflets with topics about the text. After a short preparation the exam starts with a short presentation using chalk for drawing and derivations. The student also answers questions raised during the exam. | | | | | |
|  | | | | |
| 17. List of readings  [1] N. Bronstein - K. A. Szemengyajev: Matematikai zsebkönyv , Műszaki Könyvkiadó, Budapest, 1987. | | | | | |
|  | | | | |
| 18. Recommended texts, further readings   1. Peter Atkins, Julio de Paula: Physical Chemistry, W. H. Freeman and Company, New York, 2010. | | | | | |
|  | | | | |
| **Date** | 13 April, 2017 | **Prepared by** |  | | |
| Sándor KUNSÁGI-MÁTÉ, PhD  responsible lecturer | | |
|  | | | | |
| **Endorsed by** | | |  | | |
| Dr. László Kollár, DSc program supervisor | | |