Course description

Department/Unit /	KCH / SWMOS			**Academic Year**	2016/2017
Title	Molecular Structure Modelling Software			**Type of completion**	Pre-Exam Credit
Accredited/Credits	Yes, 3 Cred.			**Type of completion**	Oral
Number of hours	Přednáška 1 [Hours/Week] Cvičení 1 [Hours/Week]				
Occ/max	Status A	Status B	Status C	**Course credit prior to**	NO
Summer semester	0 / 0	0 / 0	0 / 0	**Counted into average**	NO
Winter semester	0 / 0	6 / -	0 / 0	**Min. (B+C) students**	not determined
Timetable	Yes			**Repeated registration**	NO
Language of instruction	Czech			**Semester taught**	Winter semester
Substituted course	None			**Internship duration**	0
Preclusive courses	N/A				
Prerequisite	N/A				
Informally recommended courses	N/A				
Courses depending on this Course	N/A				

Course objectives:

The subject clarifies creation of 2D and 3D structures, especially of organic molecules, by means of Hyperchem 8.

Requirements on student

Ability to use HyperChem 8 at middle level, working on tasks during semester.

Evaluation of the subject as well as the exam grading is made according to the articles No 31 - 33 in the Regulations on Study and Examinations University of Ostrava.

Content

1. Basic drawing and editing techniques, creating small molecules
2. Polymers, proteins, nucleic acids
3. Optimalization of structure, energy of molecules
4. Molecules in water solution - function periodic box
5. Searching of conformations
6. Simulated anealing
7. Orbitals
9. Complexes
10. Vibrational spectrum
11. Excitated states and electronic spectrum
12. - 13. Practical tasks

Prerequisites - other information about course preconditions

none

Competences acquired

The students know theoretical bases of modelling software of chemical structure. They can use software HyperChem on the base level.

Fields of study

Guarantors and lecturers

- **Guarantors:** Mgr. Martin Mucha, Ph.D.
- **Lecturer:** Mgr. Martin Mucha, Ph.D.
- **Tutorial lecturer:** Mgr. Martin Mucha, Ph.D.

Literature

- **Recommended:** Hehre, W et al. *A Brief guide to Molecular Mechanics and Quantum Chemical Calculations, Irvine, Wavefunction Inc. 1998.*.

Time requirements

Activities	Time requirements for activity [h]
Being present in classes	26
Self-tutoring	13
Preparation for a credit test	26
Consultation of work with the teacher/tutor (incl. electronic)	10
Total:	**75**

assessment methods

professional knowledge

Continuous analysis of student´s achievements

teaching methods

professional knowledge

Computer-based tutoring

Individual tutoring

Monologic (explanation, lecture, briefing)

learning outcomes

professional knowledge - knowledge resulting from the course:

The students know theoretical bases of modelling software of chemical structure. They can use software HyperChem on the base level.

Course is included in study programmes:

Study Programme	Type of	Form of	Branch	Stage	St. plan v.	Year	Block	Status	R.year	R.
Chemistry	Postgraduate Master	Full-time	Analytical Chemistry of Solid Phase	1	2013	2016	Povinně volitelné předměty	B	2	ZS
Chemistry	Postgraduate Master	Full-time	Teaching for Secondary Schools - Single-Specialization Chemistry	1	2	2016	Povinně volitelné předměty	B	2	ZS
Chemistry	Postgraduate Master	Full-time	Teaching for Secondary Schools - Single-Specialization Chemistry	1	2015	2016	Povinně volitelné předměty	B		ZS