Course description

Department/Unit /	UOCHT / C042A			**Academic Year**	2022/2023
Title	Organic Dyes I			**Type of completion**	Examination
Accredited/Credits	Yes, 5 Cred.			**Type of completion**	Combined
Number of hours	Lecture 3 [HRS/WEEK]				
Occ/max	Status A	Status B	Status C	**Course credit prior to**	No
Summer semester	0 / -	0 / -	0 / -	**Counted into average**	YES
Winter semester	0 / -	0 / -	0 / -	**Min. (B+C) students**	not determined
Timetable	Yes			**Repeated registration**	NO
Language of instruction	English			**Semester taught**	Winter semester
Optional course	Yes			**Internship duration**	0
Evaluation scale	A|B|C|D|E|F				
No. of hours of on-premise					
Auto acc. of credit	No				
Periodicity	every year				
Specification periodicity					
Substituted course	KTOL/C042A				
Preclusive courses	N/A				
Prerequisite courses	N/A				
Informally recommended courses	N/A				
Courses depending on this Course	N/A				

Course objectives:

The student will learn theory of light (velocity and energy of light, wave and corpuscular properties of light), Schrödinger equation (models of exact solution for hydrogen atom, harmonic oscillator and rigid rotator), atomic and molecular orbitals, electronic absorption spectra, relationships between structure and colour of polyatomic molecules and objective evaluation of colour.

Requirements on student

examination

Content

Light: velocity and energy of light, wave properties of light, corpuscular properties of light
Schrödinger equation and its derivation, free particle, particle in potential box
Other models giving Schrödinger equation easy to solve, hydrogen atom, harmonic oscillator, rigid rotator
Solution to Schrödinger equation for simple molecules, chemical bond theory approximation, multi-electron atoms, hydrogen molecule and its ion
Atomic and molecular orbitals, hybridised AO, types of MO's (sigma, pi, n, pi*, sigma*), electron states (configuration interaction, Slater determinant)
Quantum-chemical calculation methods, precision of quantum-chemical calculations, further approximations, semi-empirical methods, Hückel's method (HMO)
Electronic absorption spectra, origin of spectra, types of transitions, energy of electron transition types pi pi* and n pi*, intensity and shape of absorption bands
Classification of organic chromogens, historical development of theory of colour, types of chromogens
Relationships between structure and colour of polyatomic molecules, basic rules of colour, absorption spectra of aromatic azo compounds
Quantum-chemical PPP method, its principles, assignment of tasks, treatment of results by bond orders, charges, spectra)
Seminar (3 hrs) - computer program PISYSTEM

Colour vision, description of human eye, rods and cones, colour vision
Objective evaluation of colour, properties of colours, colour coordinates RGB and XYZ, colour triangle, objective evaluation of colour
Optical brightening agents (OBA), physical principles of action, luminescence, structural classes of OBA, selected syntheses of OBA

Prerequisites - other information about course preconditions

Basic knowledge of organic chemistry.

Competences acquired

The student will be instructed on basics of quantum physics and relationships between structure and colour of organic molecules.

Fields of study

Guarantors and lecturers

- **Guarantors:** prof. Ing. Radim Hrdina, CSc. (100%)
- **Lecturer:** prof. Ing. Radim Hrdina, CSc. (100%)

Literature

- **Basic:** Calvert J. G., Pitts J. N. Jr. *Photochemistry, 1966 J. Wiley, N.Y.*.

Time requirements

All forms of study

Activities	Time requirements for activity [h]
Participation in classes	42
Total:	**42**

Teaching methods

Monologic (reading, lecture, briefing)

Assessment methods

Oral examination

Course is included in study programmes: