Table 5.2 Course specification

Type and level of studies: Master of Science Degree

Course name: Spectroscopic and diffraction methods in biochemistry

Course status: elective

Number of ECTS credits:6

Requirement: none

Course aim

The goal ofthe course is acquiring profound theoretical and practical knowledge of UV VIS and infra-red molecular spectroscopy. Also, gainingtheoretical knowledge of single crystal X-ray diffraction phenomena, and practical skillsneeded for crystal structure determination.

Course outcome

After successfully completing the course, the student is able to:(1) apply the acquired broad knowledge of the relevant topics of UV VIS and IR spectroscopy to improve their master thesis and the overall future chemical education.(2) Demonstrate knowledge of single crystal X-ray diffraction methods with aim to crystal structure determination; (3) Validate and interpret results of structural analysis.

Course content

Theory

Oscillatoryandoscillatory-rotational spectra ofmolecules.Spectra in theIR region. Ramanspectroscopy. The electronic spectraof molecules. Spectrain the visibleandUV range.Geometry of X-ray diffraction. Relationship between electron density and structure factor. Phase problem.Sources of X-rays. Diffraction data collection and reduction. Crystal structure determination. Geometrical analysis of the structural model and interpretation of the results. Crystallographic databanks.

Practice: Practical classes, OFT, SRW

The application ofinfraredspectroscopy for theidentification ofcompoundsandstructural analysis. IRspectroscopyin quantitative analysis. Work on four-circle diffractometer. Use of crystallographic programs for solution, refinement and validation of crystal structure models. Use of Cambridge Crystallographic Database.

Literature

1. W. Clegg, X-raycrystallography, 2nd ed., Oxford University Press, Oxford, 2015.
2. J.P. Glusker, K.N. Trueblood, Crystal structure analysis – A primer, 3rd ed., Oxford University Press, Oxford,2010.
3. J.D. Graybeal, Molecular Spectroscopy, McGraw-Hill,New York, 1988

Number of classes of active teaching				Other classes
Lectures:3	Practice:2	OFT:	SRW:	

Teaching methods

Lectures, practical teaching, problem sets, discussions, seminars.

Assessment of knowledge (maximum of 100 points)

Pre-exam obligations	**Points**	**Final exam**	**points**
activity during lecture classes	**5**	written exam	*20*
practical teaching	**20**	oral exam	25
seminars	**30**		