Study Programme: Master Academic Studies in Chemistry

Course Unit Title: Crystal Structure Determination

Course Unit Code: IHN-515

Name of Lecturer(s): Assistant professor Marko Rodić

Type and Level of Studies: Master of Science Degree

Course Status (compulsory/elective): Elective

Semester (winter/summer): Winter

Language of instruction: English

Mode of course unit delivery (face-to-face/distance learning): Face-to-face

Number of ECTS Allocated: 6

Prerequisites: None

Course Aims:

Obtaining knowledge on fundamentals of single crystal X-ray diffraction and advanced knowledge of practical steps in crystal structure determination.

Learning Outcomes:

After successfully completing the course, the student is able to:

Demonstrate knowledge of single crystal X-ray diffraction methods; experimentally perform diffraction experiment; determine and refine crystal structure; validate and interpret results of structural analysis; use Cambridge Structural Database.

Syllabus:

Theory

geometry of X-ray diffraction. Braggs law. Reciprocal lattice and Evald construction.Relationship between electron density and structure factor. Four circle diffractometer. Diffraction data collection and reduction. Determination of crystal system, unit cell and space group. Solutions to the phase problem. Completing and refinement of crystal structure model. Interpretation of results. Absolute structure determination. Crystallographic information file. Crystallographic databanks. Presentation of results.

Practice

Determination of crystal density. Selection and centering of crystalline specimen. Work on for-circle diffractometer. Use crystallographic programs form solution, refinement and validation of crystal structure models. Use of Cambridge Crystallographic Database. Presentation of theresults.

Required Reading:

1. W. Clegg, X-ray Crystallography, 2nd ed., Oxford University Press, 2015.
2. P. Müller (Ed.), Crystal Structure Refinement, Oxford University Press, 2006

Weekly Contact Hours:	**Lectures:** 2 (30)	**Practical work:** 3 (45)

Teaching Methods:

Lectures, laboratory work, desk study projects, seminar(s)

Knowledge Assessment (maximum of 100 points): 100

Pre-exam obligations	points	**Final exam**	points
Active class participation	5	written exam	20
Practical work	20	oral exam	25
Seminar(s)	30		