

Syllabus

for course at advanced level

Structure Analysis by Diffraction
Strukturanalys med diffraktion

**7.5 Higher Education
Credits**
7.5 ECTS credits

Course code:	KZ8013
Valid from:	Autumn 2014
Date of approval:	2013-11-18
Department	Department of Materials and Environmental Chemistry
Main field:	Chemistry
Specialisation:	A1F - Second cycle, has second-cycle course/s as entry requirements

Decision

This syllabus has been approved by the Board of the Faculty of Science at Stockholm University.

Prerequisites and special admittance requirements

Course structure

Examination code	Name	Higher Education Credits
MOM1	Theory	4
MOM2	Laboratory Exercises	3.5

Course content

a. The course covers basic crystallographic theory for describing structures of solid materials, in real as well as reciprocal space, and Ewald construction. Various types of radiation sources, and their pros and cons for different types of study. Basic group theoretical concepts for description of crystalline materials. Introduction to Fourier series and some essential difficulties deriving from incomplete information in diffraction data. Some methods for overcoming the so-called crystallographic phase problem: heavy atom methods, and an introduction to "direct methods". Least-squares refinement of structure models, and calculation of geometric parameters. Collection of diffraction data and interpretation of such data, using crystallographic program packages for inorganic materials and organic and metal-organic small molecule structures. Analysis and presentation of structure models.

b. The course includes the following two elements:

1. Theory 4 credits
2. Laboratory exercises 3.5 credits

Learning outcomes

It is expected that the student after taking the course will be able to:

- Demonstrate basic theoretical and experimental knowledge in structure determination of solid materials, using diffraction methods.
- Describe basic symmetry properties of solid 3-dimensional materials, especially in relation to structure determination using single-crystal methods.
- Interpret measurement data and use group theoretical models to describe solid materials
- Demonstrate basic understanding of difficulties in transforming diffraction data (Fourier representation) to structure models in real space, and commonly employed methods for overcoming these difficulties.

Education

The education consists of lectures, group work, computational training and laboratory exercises. Participation in the practical laboratory work and group education associated with this is compulsory. After consultation with the relevant teacher, an examiner may rule that a student is not obliged to participate in certain compulsory education, if there are special grounds for this.

Forms of examination

a. Measurement of knowledge takes place through:

- Written and/or oral examination

b. Grading is carried out according to a 7-point scale related to learning objectives:

A = Excellent, B = Very Good, C = Good, D = Satisfactory,

E = Sufficient Fx = Fail F = Fail.

c. Grading criteria for the course will be distributed at the start of the course.

d. A minimum grade of E is required to pass the course, together with:

- completion of all practical laboratory work, followed by its presentation and award of a "Sufficient" grade

e. Students who fail to achieve a pass grade in an ordinary examination have the right to take at least further four examinations, as long as the course is given. The term "examination" here is used to denote also other compulsory elements of the course. Students who have achieved a pass grade on an examination may not retake this examination in order to attempt to achieve a higher grade. Students who have failed to reach a pass grade on two occasions have the right to request that a different teacher be appointed to set the grade of the course. A request for such appointment must be sent to the departmental board.

Interim

Students may request that the examination is carried out in accordance with this syllabus even after it has ceased to apply. This right is limited, however, to a maximum of three occasions during a two-year-period after the end of giving the course. A request for such examination must be sent to the departmental board.

Limitations

The course may not be included in a degree together with the course KE3980 (Structural analysis by diffraction, level 2, 5 credits) or with the diffraction part of KE3680 (Structural analysis by diffraction and electron microscopy) or other equivalents.

Required reading

Course literature is decided by the departmental board and is described in an appendix to the syllabus.