“Structural analysis with diffraction”, KZ8013, 7.5hp

The course consist of:

Lectures describing the theory of crystallography enough well for students to be able to solve the practical problems connected with determination of unknown structures from single crystals using diffraction methods.

Calculation exercises connected to each chapter in the lecture notes. It is strongly recommended that one should be able to solve and even more important, understand, all of the different problems present in these exercises. Some of them may need rather much work and may not have an easy short “answer”.

It is strongly recommended to use some numerical computer program for solving many of the calculation exercises.

Three different projects:

1. The first project aims at getting used to searching structural information in databases and presenting it with some suitable crystallographic drawing programs . ***Each student will have an individual project that should be described with an oral presentation***. The presentations should preferably focus on solving chemical problems with the use of crystallographic data.
2. The second project aims at getting used to all steps and procedures in a complete structure investigation: As this project is common to all students you may cooperate as you wish, but an ***individual written report*** should be handed in.
3. The third project aims at deepened knowledge to all steps and procedures of a complete structural investigation of a more advanced character than project two. ***Each student receives an individual subject/substance***. A few crystals may be measured if time allows, otherwise “old data” will be used. Cooperate as you wish, but ***each student should do an individual oral presentation.*** Power point presentations (or similar) is encouraged.

Finally there are four **exercises** that should be reported either in ***seminar*** or as ***written reports***.

1. “Space group determination exercise” using systematic reflection conditions, symmetries in reciprocal space and intensity statistics.
2. ”Structure solution from heavy atom data”, by interpretation of Patterson map.
3. “Direct methods structure solution and complete refinement of a small molecule structure”
4. “Direct methods structure solution and complete refinement of a metal complex”

Literature

The recommended literature is:

International Tables For Crystallography: Space Group Symmetry, Brief Teaching Edition of Volume A

Edited by Theo Hahn, Kluwer Academic Publishers Group (2001), Fifth revised edition (2005)

ISBN-13: 9780792365914

Available e.g. at http://www.bokus.com/bok/9780470689110/international-tables-for-crystallography-v-a/

In addition some locally produced material, “Lecture Notes for Structural Analysis with Diffraction” will be available.

Schedule: “Strukturanalys med diffraktion”, KZ8013, 7.5hp. [20-jan-2025 ... 19-feb-2025]

F = Föreläsning/lektion/lecture/lesson; **L**=Lab exercise, **P=**Presentation, **R**=calculation exercise, **S**=Seminar.

The language will be English if necessary. Most of the software used will be available for download to your own laptop computer.

Date	10-12	13.15-16	Teacher
20-jan	F1: Math repetition and introduction to Octave.		**Lasse**
21	F2: Crystals, X-ray sources, absorption.	L1: Start of **project 1.**	**Ken**
22	F3: Scattering in crystals, Laue and Ewald.		**Ken**
23	F4: Point groups and space groups-I.	**R1.**	**Ken**
24		**P1**: Oral presentation of project 1.	
27	F5: Point groups and space groups-II. Data collection-I, spacegr. det. and refl. cond.	L2: Space group determination exercise.	**Ken**
28	F6: Fourier series, electron density and Patterson map and interpretation. Start of **project 2.**	L3: Structure solution by interpretation of Patterson map.	**Lasse**
29	F7: Direct methods-I, SHELX suite.	**R2**	**Lasse**
30	Preparation for seminar	**S1** – lab (2,3) seminar.	
31			
3-feb	F8: Direct methods-II	L4: Structure solution of TKLBFA.	**Lasse**
4	F9: Refinement of crystal structures, restraints	L5: Structure solution of Cu-komplex.	**Lasse**
5	F10: Data collection-II, twinning, Flack.	L6: Data coll., RT, cryo, **project 3.**	**Lasse**
6	Preparation for seminar	**S2** – lab (4,5) seminar.	
7			
10	F11: Interpretation of results, cif format	Project 3	**Lasse**
11	F12: Electron diffraction.	Project 3	**Lasse**
12	F13: Synchrotron and neutron scatt.	Project 3	**Lasse**
13	Project 3	Project 3	
14			
17		**P2**: Oral presentation of project 3.	
18			
19		**Examination**	
20	*Next course begins... (powder diffraction perhaps?)*		
21			

Teachers in the course:

Ken Inge Andrew, Lars Eriksson and Walter Wong