Information about the course "Structural analysis with diffraction", KZ8013, 7.5hp

The course consists 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 five **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. "Direct methods structure solution and complete refinement of a small molecule structure"
3. Calculation exercise-1 (selected from the lecture notes)
4. Calculation exercise-2 (selected from the lecture notes)
5. Calculation exercise-3 (selected from the lecture notes)

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. The lecture notes contains material connected to each lecture. It is however not a "printout" of the lectures but should be regarded as a complement to the lectures. In addition to each chapter in the lecture notes, there are some exercises appended.

Schedule for the course "Strukturanalys med Diffraktion", KZ8013, 7.5hp. [15-jan-2018 ... 14-feb-2018]

F = Föreläsning/lektion/lecture/lesson; **L**=Laboration/exercise, **P**=Presentation, **R**=Räkneövning/calculation exercise. All lectures and calculation exercises as well as computer exercises will take place in the combined literature / computer room C513. The language will be English if necessary. Most of the software used (except databases) will be available for download to your own laptop computer.

Date	9.15-12	13.15-16
15-jan		F1: Crystals, X-ray sources, absorption and absorption corrections. L1: Start of project 1, CSD, ICSD, PDB, PDF4,...
16		F2: Math repetition and introduction to Octave.
17	R1: Calculation exercise 1	F3: Scattering in crystals, Laue and Ewald.
18		F4: Point groups and space groups-I.
19		P1: Oral presentation of project 1
22		F5: Point groups and space groups-II. Data collection-I, spacegr. det. and refl. cond.
23	R2: Calculation exercise 2	F6: Fourier series and electron density. L2: Space group determination exercise.
24		
25		F7: Structure solution, heavy atom methods. L3: Introduction to SHELX and **project 2**
26		
29		F8: Direct methods, SHELXS, SHELXD, SHELXT L4: Structure solution by direct methods
30		F9: Powder diffraction, small angle scattering
31	R3: Calculation exercise 3	F10: Data collection-II, effects of environment. L5: Data collection, RT, **start of project 3**
1-feb	Project 3	F11: Refinement of crystal structures, restraints L6: Data collection, Cryo, project 3
2		
5	Project 3	Seminar (space groups, direct methods and R1-R3)
6	Project 3	F12: Interpretation of results, cif format
7	Project 3	F13: Flack x, twinning, synchrotron and neutron scatt.
8	Project 3	Project 3
9		
12		P2: Oral presentation of project 3
13		
14	**Examination (09.15- 14.15)**	
15	*Next course begins... (Neutrons perhaps?)*	
16		