



KD1070 Molecular Structure 6.0 credits

Molekylär struktur

This is a translation of the Swedish, legally binding, course syllabus.

If the course is discontinued, students may request to be examined during the following two academic years

Establishment

Course syllabus for KD1070 valid from Spring 2022

Grading scale

A, B, C, D, E, FX, F

Education cycle

First cycle

Main field of study

Technology

Language of instruction

The language of instruction is specified in the course offering information in the course catalogue.

Intended learning outcomes

1. to formulate, model, and solve problems in selected simple quantum mechanical systems, to describe and analyze atomic and molecular features on a quantum mechanical ground and to identify and exemplify those different factors that contribute to chemical binding and intermolecular interactions and their role in the properties of materials.
2. to describe and explain basic spectroscopic principles and their role and influence in spectroscopic experiments and tools and to calculate and explain the results obtained by spectroscopic or structural-chemistry experiments and to relate those to molecular and phase properties

in order to

- to be able to independently identify, explain, and predict the various environmental impacts of particular chemicals and to motivate a sustainable use of those
- as a professional, to be able to identify and investigate problems related to molecular and material properties and spectroscopic methods

Course contents

- Elementary quantum mechanics
- Electronic structure of atoms, atomic orbitals, the basis for the periodic system
- Chemical bonding, molecular orbitals, hybridization, singlet and triplet states, applications of chemical bonding in organic, inorganic, and biological molecules
- Background to modern quantum chemical methods
- Intermolecular interactions, gases-liquids-liquid crystals-solids, supermolecular structures, e.g. biomembranes
- Spectroscopical methods such as IR, Raman, UV/VIS, NMR, MS, ESCA
- Diffraction methods
- Structural chemistry

Most of the experimental methods and the computational quantum chemistry are exemplified by laboratory and/or computer exercises.

Specific prerequisites

Examination

- LAB1 - Laboratory Work, 1.5 credits, grading scale: P, F
- TEN1 - Written exam, 4.5 credits, grading scale: A, B, C, D, E, FX, F

Based on recommendation from KTH's coordinator for disabilities, the examiner will decide how to adapt an examination for students with documented disability.

The examiner may apply another examination format when re-examining individual students.

Other requirements for final grade

Examination 4,5 credits

Laboratory work 1,5 credits

Ethical approach

- All members of a group are responsible for the group's work.
- In any assessment, every student shall honestly disclose any help received and sources used.
- In an oral assessment, every student shall be able to present and answer questions about the entire assignment and solution.