



# KD2040 Quantum Chemistry and Spectroscopy 9.0 credits

Kvantkemi och spektroskopi

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

## Establishment

Course syllabus for KD2040 valid from Autumn 2007

## Grading scale

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

## Education cycle

Second cycle

## Main field of study

## Specific prerequisites

The basic courses in chemistry and mathematics for K.

## Language of instruction

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

## Intended learning outcomes

To provide the first practical experience and the future starting point for solving structural and dynamical problems in chemistry by applying spectroscopic experiments and quantum chemical calculations.

## Course contents

The course consists of three parts of roughly the same length. The essential quantum mechanics that is required later is covered in the first part. The basic quantum mechanical principles and their applications to model systems once mentioned in the basic course are discussed in detail. Approximative tools such as the perturbation theory and the variation method are introduced.

Basic molecular spectroscopy is treated in the second part of the course. Different kinds of interaction between electromagnetic radiation and molecules are discussed which then leads to the basic principles of various optical (such as infrared and Raman) and magnetic resonance (such as NMR and ESR) spectroscopies. Time-domain spectroscopies using short pulses of radiation and applied to studies of rapid chemical dynamics are discussed. The particularly powerful nuclear magnetic resonance spectroscopy is treated in more detail in the course KD2060, NMR Spectroscopy.

Methods of quantum chemical calculations and their applications in chemistry and biochemistry are treated in the third part of the course:

- the Hartree-Fock method; theoretical background and implementation.
- Calculations of molecular properties; energies, molecular geometries, vibrational spectra and electrostatic potentials.
- Quantum chemical studies of intermolecular interactions; chemical reactivity and biological activity.

This part of the course includes two quantum-chemical calculation assignments where a modern quantum chemical software package is used for computing molecular properties and for analysing chemical problems.

## Course literature

1. A. I. M. Rae: Quantum Mechanics, 3rd ed., Institute of Physics, 1993.
2. A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Dover, 1995.

## Examination

- TEN1 - Examination, 6.0 credits, grading scale: A, B, C, D, E, FX, F
- LAB1 - Laboratory Work, 3.0 credits, grading scale: P, 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.

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

## Other requirements for final grade

1. Combined written/oral examination; voluntary student seminars may replace the oral part, 6 credits.
2. Fulfilled laboratory course and calculation assignment, 3 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.