

# **Physical Chemistry, Spectroscopy**

Fysikalisk kemi, spektroskopi 6 credits

Programme course

NKEB09

Valid from: 2023 Spring semester

Determined by	Main field of study	
Board of Studies for Chemistry, Biology and Biotechnology	Chemistry	
Date determined	Course level	Progressive specialisation
2022-08-31	First cycle	G1X
Revised by	Disciplinary domain	
	Natural sciences	
Revision date	Subject group	
	Chemistry	
Offered first time	Offered for the last time	
Spring semester 2008		
Department	Replaced by	
Institutionen för fysik, kemi och biologi		

## Course offered for

- Bachelor's Programme in Chemical Biology
- Bachelor's Programme in Chemistry Molecular Design

## **Prerequisites**

General Chemistry, Organic Chemistry, Biochemistry, Physical Chemistry, Thermodynamics, Mathematics

## Intended learning outcomes

The course aims to confer knowledge in physical chemistry within the areas kinetics, quantum mechanics and molecular spectroscopy and skills in problem solving and laboratory tasks within the areas listed in the course contents below. After successfully completed course the course participant will be able to:

- understand the basic principles underlying the physical processes covered in the course
- describe and discuss the physical phenomena as well as the kinetic and spectroscopic instruments and measurement techniques
- account for, explain and exemplify the theory
- perform calculations for and solve problems within the course content area.
- analyse and apply the acquired facts and skills on complex physical processes
- conclude whether obtained results are reasonable and reflect over fundamental physical-chemistry problems in science, nature and society
- work with physical-chemistry problems solitarily and in groups
- analyse, compile and account for the laboratory exercise results in laboratory reports.

## Course content

Lectures, lessons and laboratory exercises cover the following areas: Kinetics: rate equations and their integration, reaction order, half life, mechanisms, catalysis, photochemistry, techniques for measuring fast reactions, flow, flash and relaxation methods, activation energies and molecular reaction dynamics. Quantum mechanics: basic quantum-mechanical concepts, particle-in-a-box, harmonic and anharmonic oscillator, rotation on a ring and on a sphere, the hydrogen atom, plus elementary introduction to many-electron atomic and molecular electron structure. Spectroscopy: interaction between electromagnetic radiation and matter by absorption and emission, fluorescence and phosphorescence, lasers, rotational, vibrational and electron spectroscopic methods such as microwave, infrared, visible/UV, X-ray photoelectron and magnetic resonance spectroscopy.



## Teaching and working methods

The theory is presented during the lectures. Problem solving is practised during the lessons. In the laboratory exercises fundamental laboratory techniques and moments connected to the theory and problem solving are practised. The laboratory exercises, whose laboratory exercise instructions and safety rules must be studied prior to the exercise, are mandatory. Written reports are handed in within five workdays from the laboratory exercise occasion. For the laboratory exercises special premises are required.

## Examination

LAB1	Laboratory work	1.5 credits	U, G
TEN <sub>1</sub>	Written examination	4.5 credits	U, 3, 4, 5

The problems at the written examination probes to what extent the participant fulfils the aims of the course. For approved laboratory work carried-through laboratory exercises and approved reports are required. For grade 3, 4 and 5, respectively, on the course, grade 3, 4 and 5, respectively, on the written exam together with grade G on the laboratory work are required.

## Grades

Four-grade scale, LiU, U, 3, 4, 5



## Other information

Supplementary courses: Materials Chemistry, Chemical Bonding, Computational Chemistry, Nanochemistry A and B, Coordination Chemistry, Physical-Organic Chemistry, Biological Measurements.

### About teaching and examination language

The teaching language is presented in the Overview tab for each course. The examination language relates to the teaching language as follows:

- If teaching language is "Swedish", the course as a whole could be given in Swedish, or partly in English. Examination language is Swedish, but parts of the examination can be in English.
- If teaching language is "English", the course as a whole is taught in English. Examination language is English.
- If teaching language is "Swedish/English", the course as a whole will be taught in English if students without prior knowledge of the Swedish language participate. Examination language is Swedish or English depending on teaching language.

#### Other

The course is conducted in a manner where both men's and women's experience and knowledge are made visible and developed.

The planning and implementation of a course should correspond to the course syllabus. The course evaluation should therefore be conducted with the course syllabus as a starting point.

The course is campus-based at the location specified for the course, unless otherwise stated under "Teaching and working methods". Please note, in a campus-based course occasional remote sessions could be included.

If special circumstances prevail, the vice-chancellor may in a special decision specify the preconditions for temporary deviations from this course syllabus, and delegate the right to take such decisions.



## **Common rules**

## Course syllabus

A syllabus must be established for each course. The syllabus specifies the aim and contents of the course, and the prior knowledge that a student must have in order to be able to benefit from the course.

## **Timetabling**

Courses are timetabled after a decision has been made for this course concerning its assignment to a timetable module.

## Interruption in and deregistration from a course

The LiU decision, Guidelines concerning confirmation of participation in education (Dnr LiU-2020-02256), states that interruptions in study are to be recorded in Ladok. Thus, all students who do not participate in a course for which they have registered must record the interruption, such that the registration on the course can be removed. Deregistration from or interrupting a course is carried out using a web-based form Forms

## Cancelled courses and changes to the course syllabus

Courses with few participants (fewer than 10) may be cancelled or organised in a manner that differs from that stated in the course syllabus. The Dean is to deliberate and decide whether a course is to be cancelled or changed from the course syllabus.

## Guidelines relating to examinations and examiners

For details, see Guidelines for education and examination for first-cycle and second-cycle education at Linköping University, Dnr LiU-2020-04501 (http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592).

An examiner must be employed as a teacher at LiU according to the LiU Regulations for Appointments, Dnr LiU-2021-01204 (https://styrdokument.liu.se/Regelsamling/VisaBeslut/622784). For courses in second-cycle, the following teachers can be appointed as examiner: Professor (including Adjunct and Visiting Professor), Associate Professor (including Adjunct), Senior Lecturer (including Adjunct and Visiting Senior Lecturer), Research Fellow, or Postdoc. For courses in first-cycle, Assistant Lecturer (including Adjunct and Visiting Assistant Lecturer) can also be appointed as examiner in addition to those listed for second-cycle courses. In exceptional cases, a Part-time Lecturer can also be appointed as an examiner at both first- and second cycle, see Delegation of authority for the Board of Faculty of Science and Engineering.



## Forms of examination

### **Principles for examination**

Written and oral examinations and digital and computer-based examinations are held at least three times a year: once immediately after the end of the course, once in August, and once (usually) in one of the re-examination periods. Examinations held at other times are to follow a decision of the faculty programme board.

Principles for examination scheduling for courses that follow the study periods:

- courses given in VT1 are examined for the first time in March, with reexamination in June and August
- courses given in VT2 are examined for the first time in May, with reexamination in August and January
- courses given in HT1 are examined for the first time in October, with reexamination in January and August
- courses given in HT2 are examined for the first time in January, with reexamination in March and in August.

The examination schedule is based on the structure of timetable modules, but there may be deviations from this, mainly in the case of courses that are studied and examined for several programmes and in lower grades (i.e. 1 and 2).

Examinations for courses that the faculty programme board has decided are to be held in alternate years are held three times during the school year in which the course is given according to the principles stated above.

Examinations for courses that are cancelled or rescheduled such that they are not given in one or several years are held three times during the year that immediately follows the course, with examination scheduling that corresponds to the scheduling that was in force before the course was cancelled or rescheduled.

When a course, or a written examination (TEN, DIT, DAT), is given for the last time, the regular examination and two re-examinations will be offered. Thereafter, examinations are phased out by offering three examinations during the following academic year at the same times as the examinations in any substitute course. If there is no substitute course, three examinations will be offered during re-examination periods during the following academic year. Other examination times are decided by the faculty programme board. In all cases above, the examination is also offered one more time during the academic year after the following, unless the faculty programme board decides otherwise. In total, 6 re-examinations are offered, of which 2 are regular re-examinations. In the examination registration system, the examinations given for the penultimate time and the last time are denoted.

If a course is given during several periods of the year (for programmes, or on different occasions for different programmes) the faculty programme board or boards determine together the scheduling and frequency of re-examination occasions.



#### Retakes of other forms of examination

Regulations concerning retakes of other forms of examination than written examinations and digital and computer-based examinations are given in the LiU guidelines for examinations and examiners,

http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592.

#### Course closure

For Decision on Routines for Administration of the Discontinuation of Educational Programs, Freestanding Courses and Courses in Programs, see DNR LiU-2021-04782. After a decision on closure and after the end of the discontinuation period, the students are referred to a replacement course (or similar) according to information in the course syllabus or programme syllabus. If a student has passed some part/parts of a closed program course but not all, and there is an at least partially replacing course, an assessment of crediting can be made. Any crediting of course components is made by the examiner.

### **Registration for examination**

In order to take an written, digital or computer-based examination, registration in advance is mandatory, see decision in the university's rule book <a href="https://styrdokument.liu.se/Regelsamling/VisaBeslut/622682">https://styrdokument.liu.se/Regelsamling/VisaBeslut/622682</a>. An unregistered student can thus not be offered a place. The registration is done at the Student Portal or in the LiU-app during the registration period. The registration period opens 30 days before the date of the examination and closes 10 days before the date of the examination. Candidates are informed of the location of the examination by email, four days in advance.

#### Code of conduct for students during examinations

Details are given in a decision in the university's rule book: http://styrdokument.liu.se/Regelsamling/VisaBeslut/622682.

#### Retakes for higher grade

Students at the Institute of Technology at LiU have the right to retake written examinations and digital and computer-based examinations in an attempt to achieve a higher grade. This is valid for all examination components with code "TEN", "DIT" and "DAT". The same right may not be exercised for other examination components, unless otherwise specified in the course syllabus.

A retake is not possible on courses that are included in an issued degree diploma.

#### **Grades**

The grades that are preferably to be used are Fail (U), Pass (3), Pass not without distinction (4) and Pass with distinction (5).

- Grades U, 3, 4, 5 are to be awarded for courses that have written or digital examinations.
- Grades Fail (U) and Pass (G) may be awarded for courses with a large degree of practical components such as laboratory work, project work and



group work.

• Grades Fail (U) and Pass (G) are to be used for degree projects and other independent work.

## **Examination components**

The following examination components and associated module codes are used at the Faculty of Science and Engineering:

- Grades U, 3, 4, 5 are to be awarded for written examinations (TEN) and digital examinations (DIT).
- Examination components for which the grades Fail (U) and Pass (G) may be awarded are laboratory work (LAB), project work (PRA), preparatory written examination (KTR), digital preparatory written examination (DIK), oral examination (MUN), computer-based examination (DAT), home assignment (HEM), and assignment (UPG).
- Students receive grades either Fail (U) or Pass (G) for other examination components in which the examination criteria are satisfied principally through active attendance such as tutorial group (BAS) or examination item (MOM).
- Grades Fail (U) and Pass (G) are to be used for the examination components Opposition (OPPO) and Attendance at thesis presentation (AUSK) (i.e. part of the degree project).

In general, the following applies:

- Mandatory course components must be scored and given a module code.
- Examination components that are not scored, cannot be mandatory. Hence, it is voluntary to participate in these examinations, and the voluntariness must be clearly stated. Additionally, if there are any associated conditions to the examination component, these must be clearly stated as well.
- For courses with more than one examination component with grades U,3,4,5, it shall be clearly stated how the final grade is weighted.

For mandatory components, the following applies (in accordance with the LiU Guidelines for education and examination for first-cycle and second-cycle education at Linköping University,

http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592):

• If special circumstances prevail, and if it is possible with consideration of the nature of the compulsory component, the examiner may decide to replace the compulsory component with another equivalent component.

For possibilities to alternative forms of examinations, the following applies (in accordance with the LiU Guidelines for education and examination for first-cycle and second-cycle education at Linköping University, <a href="http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592">http://styrdokument.liu.se/Regelsamling/VisaBeslut/917592</a>):

• If the LiU coordinator for students with disabilities has granted a student the right to an adapted examination for a written examination in an examination hall, the student has the right to it.



- If the coordinator has recommended for the student an adapted examination or alternative form of examination, the examiner may grant this if the examiner assesses that it is possible, based on consideration of the course objectives.
- An examiner may also decide that an adapted examination or alternative form of examination if the examiner assessed that special circumstances prevail, and the examiner assesses that it is possible while maintaing the objectives of the course.

### Reporting of examination results

The examination results for a student are reported at the relevant department.

### **Plagiarism**

For examinations that involve the writing of reports, in cases in which it can be assumed that the student has had access to other sources (such as during project work, writing essays, etc.), the material submitted must be prepared in accordance with principles for acceptable practice when referring to sources (references or quotations for which the source is specified) when the text, images, ideas, data, etc. of other people are used. It is also to be made clear whether the author has reused his or her own text, images, ideas, data, etc. from previous examinations, such as degree projects, project reports, etc. (this is sometimes known as "self-plagiarism").

A failure to specify such sources may be regarded as attempted deception during examination.

#### Attempts to cheat

In the event of a suspected attempt by a student to cheat during an examination, or when study performance is to be assessed as specified in Chapter 10 of the Higher Education Ordinance, the examiner is to report this to the disciplinary board of the university. Possible consequences for the student are suspension from study and a formal warning. More information is available at Cheating, deception and plagiarism

## Regulations (apply to LiU in its entirety)

The university is a government agency whose operations are regulated by legislation and ordinances, which include the Higher Education Act and the Higher Education Ordinance. In addition to legislation and ordinances, operations are subject to several policy documents. The Linköping University rule book collects currently valid decisions of a regulatory nature taken by the university board, the vice-chancellor and faculty/department boards.

LiU's rule book for education at first-cycle and second-cycle levels is available at http://styrdokument.liu.se/Regelsamling/Innehall/Utbildning\_pa\_grund-och\_avancerad\_niva.

