UNIVERSITY OF GOTHENBURG

DEPARTMENT OF CHEMISTRY AND MOLECULAR BIOLOGY

KEM040 Physical Chemistry, 15 credits

Fysikalisk kemi, 15 högskolepoäng

First Cycle

Confirmation

This course syllabus was confirmed by Department of Chemistry and Molecular Biology on 2017-09-25 and was last revised on 2017-10-03 to be valid from 2017-10-03, autumn semester of 2017.

Field of education: Science 100%

Department: Department of Chemistry and Molecular Biology

Position in the educational system

The course is classified at the level 30-60 credits for Degree of Bachelor. Alternatively, it can be read as a freestanding course. The course replaces KEN040, and the courses cannot be counted in together for the same degree.

The course can be part of the following programmes: 1) Chemistry and learning, Master's Programme (N2KOL), 2) Master's Programme in Organic and Medicinal Chemistry (N2KEL), 3) Master's Programme in Chemistry (N2KEM), 4) Bachelor of Science Programme in Medicinal Chemistry (N1LMK), 5) Bachelor of Science Programme in Chemistry (N1KEM) and 6) Teacher Training Programme (L1LÄR)

Main field of studies	*Specialization*
Chemistry	G1F, First Cycle, has less than 60 credits in first-cycle course/s as entry requirements
Chemistry with Specialization in Medicinal Chemistry	G1F, First Cycle, has less than 60 credits in first-cycle course/s as entry requirements

Entry requirements

For admission to the course, passed course KEM011, Basic chemistry 1 (15 credits) or equivalent knowledge is required. Completed course Mathematics for natural scientists A1 (15 credits), course code MMGK11 or equivalent knowledge is strongly recommended.

Learning outcomes
On successful completion of the course the student will be able to:

Knowledge and understanding

- **decide** when quantum mechanically based or classical mechanical problem-solving are applicable to physicochemical problems,
- **explain** the concepts of
  - particle in a box, harmonic oscillator and molecular rotor,
  - Hückel, linear combination of atomic orbital (LCAO), valence-bond (VB), and molecular orbital (MO) models,
  - entropy and spontaneity in a chemical process,
  - Boltzmann distribution and canonical partition function,
  - resonance on atomic and molecular levels,
  - relationships between wave number, wavelength and frequency,
  - absorbance and emission (i.e. fluorescence, phosphorescence, spontaneous emission, and stimulated emission),
- **account for**
  - the molecular driving forces and properties that determine direction and equilibrium of a chemical reaction,
  - spectroscopic methods of measurement in molecular terms.

Competence and skills

- **analyse** problems as well as **perform** calculations in fields
  - quantum mechanics and spectroscopy with a focus on molecular translation, vibration and rotation as well as electron structure and bonding mechanisms in atoms and molecules,
  - thermodynamics and statistical mechanics with a focus on gases, liquids and solutions in equilibrium by means of the laws of thermodynamics,
  - chemical kinetics with a focus on reaction rates,
- **define** geometry and physical properties of molecules based on elementary quantum chemistry,
- **perform** physicochemical measurements as well as **interpret** results from a molecular perspective.

Judgement and approach

- **reflect on** and **discuss** physicochemical issues on the basis of scientifically based understanding of atomic and molecular processes,
- **argue** for physicochemically founded presentations of problems connected to an environmentally sustainable society and sustainable development.

The course is sustainability-related, which means that at least one of the learning outcomes clearly shows that the course content meets at least one of the University of Gothenburg's confirmed sustainability criteria.

Course content

Quantum Mechanics

- Quantum quantisation of light and particle motion. Wave-particle dualism. Uncertainty principle.
- Schrödinger equation: particle in box, harmonic oscillator, rigid rotor, tunnelling.
- Qualitative quantum mechanics.

Quantum chemistry

- Hydrogen-like systems, larger atoms.
- Lewis structures, VSEPR and VB models for molecules.
- Ionic and covalent chemical binding. Molecular orbital models as linear combination of atomic orbitals.
- Hydrogen molecular ion, hydrogen molecule, ethene, and larger molecules.
- Electronic structure calculations, particularly Hückel theory for planar conjugated hydrocarbon molecules.

Spectroscopy

- The principles of spectroscopy, properties of light, as well as connection to quantized state of atoms and molecules. Absorption, scattering, and emission. Interpretation of spectra.
- Vibration spectroscopy for diatomic molecules with the harmonic oscillator as starting point. Selection rules and procedures, anharmonicity as well as normal modes for simple polyatomic molecules.
- Rotational spectroscopy, with connection to rotational motion of simple molecules. Coupling of vibration and rotational motions.
- Electronic transitions and optical spectroscopy. The concepts of fluorescence and phosphorescence. Principle of laser. Line broadening and the concept of quenching.

- Related spectroscopic technologies and Raman scattering.

Statistical Mechanics

- Microstates, ensembles, Boltzmann distribution, partition function.
- Internal energy, entropy, free energy, thermal capacities and equilibrium constants calculated from partition functions.
- Ideal and real gases.

Thermodynamics

- Energy in the form of work and heat according to first main clause.
- Entropy and free energy according to other main clause.
- Multi-component systems, mixtures and solutions.
- Chemical potential, non-ideal systems, activity, ionic solutions, phase equilibrium, chemical equilibrium.
- Multi-phase systems and phase transitions.
- Electrochemistry.

Kinetics

- Kinetic gas theory, transport properties, movement in liquids, diffusion.
- Reaction orders, Arrhenius equation, reaction mechanisms.
- Collision theory, transition-state theory, dynamics.

Sub-courses

1. **Theory part** *(Teoridel),* 9 credits
   Grading scale: Pass with Distinction (VG), Pass (G) and Fail (U)
2. **Laboratory exercises** *(Laborationer),* 6 credits
   Grading scale: Pass (G) and Fail (U)

Form of teaching

Part 1: Lectures, calculation exercises, and/or assisted problem solving and home assignments.

Part 2: Laboratory sessions.

Language of instruction: Swedish and English
As principal rule, the course is given in Swedish but can be given completely or partly in English if the circumstances require it.

Assessment

Part 1: Examination takes place by a written in-class examination.

Part 2: Examination takes place based on active participation in laboratory sessions and laboratory reports.

If a student who has failed the same part of the examination twice wishes to change examiner before the next examination, a written application shall be sent to the department responsible for the course and shall be granted unless there are special reasons to the contrary (Chapter 6, Section 22 of Higher Education Law).

In cases where a course has been discontinued or has undergone major changes, the student shall normally be guaranteed at least three examination sessions (this number including the ordinary examination) during a period of at least one year from the last time the course was given.

Grades

The grading scale comprises: Pass with Distinction (VG), Pass (G) and Fail (U).
Part 1: For grade Pass, 50% of the maximum total score in the examination are required. For grade Pass with distinction, 75% of the maximum total score in the examination are required.

Part 2: For grade Pass, completion of laboratory work and approved laboratory reports are required for all laboratory sessions.

Final grade: For grade Pass on the whole course, grade Pass on both modules is required. For grade Pass with distinction on the whole course, grade Pass with distinction on module 1 and grade Pass on module 2 are required.

Regarding application of the ECTS scale for grade please see Vice-Chancellor decision 28/05/2007, diary nr G 8 1976/07.

Course evaluation

A course evaluation is done in relation to the intended learning outcomes and content of the course. It is performed at the end of the course through an individual written questionnaire on the virtual learning environment at University of Gothenburg. A student who participates in or has completed a course should be given possibility to anonymously express experiences of and views in the course in a course evaluation. A compilation of the course evaluation and reflections of the course coordinator should be made available for the students within reasonable time after the end of the course.