SCI PHYS 202 Physical Chemistry
Fall 2019

University College Roosevelt

PHYS SCI 202 Physical Chemistry

Fall 2019

Classroom no:	Franklin 13
Class times:	Tuesday 11:00 – 13:00 & Friday 08:45 – 10:45
Instructor:	Dr. L. de Wit
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Tel:	
Office no. & location:	Eleanor 2.08
Office hours:	by appointment

I. Track information

a) Prerequisites for this course:
   To register for this course, you must have completed the SCI PHYS 101 Introduction to Physics
b) This course serves as prerequisite for:
   SCI PHYS 202 Physical Chemistry is a possible prerequisite for both SCI PHYS 301 Advanced Physics and SCI PHYS 302 Particle Physics
c) Other courses which are relevant to this course – e.g. as part of a minor:
   Courses in the mathematics and computer science track

For further information about the track, please see the track document available on the UCR intranet.

II. Course description

The course Physical Chemistry is a 200-level course in the Physics track. The main goal of this course is to connect the microscopic world - at the level of atoms and molecules - to the macroscopic world - in terms of liters of gas - and show that macroscopic quantities such as pressure, heat capacity and entropy are determined by microscopic quantum mechanical properties like energy quantization. This course will focus on the three main areas within the field of Physical Chemistry:
1. Quantum Chemistry (concerning the structures of molecules),
2. Thermodynamics (concerning the energetics of chemical reactions), and
3. Chemical Kinetics (concerning the rates of chemical reactions).

<u>1 Quantum Chemistry</u>

The first part of the course focuses on Quantum Mechanics. It reviews Quantum Mechanics as discussed in PHYS 101: the particle-in-a-box problem and the harmonic oscillator will be discussed. We will have again a look at the solution of the Schrodinger Equation for the

Hydrogen atom. The Schrodinger Equation cannot be solved exactly in the case of multi electron atoms. This course will discuss two approximation methods; perturbation theory and the variational method. These techniques allow for a quantum mechanical discussion on electronic wave functions, atomic wave functions and molecular orbital wave functions. Finally, the course discusses chemical bonding and bonding in polyatomic molecules.

2 Thermodynamics

PHYS 202 Physical Chemistry will present a thorough discussion on thermodynamics. This part of the course starts with a discussion on the properties of gases. It will discuss partition functions and statistical thermodynamics. All macroscopic quantities such as pressure and temperature arise from molecular properties. The course continues with the laws of thermodynamics; heat, pressure-volume work, internal energy; entropy and enthalpy. Finally, we will discuss how absolute entropies can be calculated from tabulated heat capacities. The last subject is the kinetic theory of gases.

3 Chemical Kinetics

In the last weeks of the semester we will briefly look at chemical kinetics. Rate laws describe the time dependency of a chemical reaction. The course discusses how rate laws can be determined experimentally, and how one can distinguish between different reaction mechanisms.

III. Study Load

This course earns students four credits (equivalent to 7.5 ECTS). The class meets twice a week for two hours. Preparation time is approximately 10 hours per week.

IV. Course materials

a) Required books and literature:

Physical Chemistry: A Molecular Approach
Donald A. McQuarrie and John Simon
published by University Science Books (1997)
ISBN-number is 0-935702-99-7

b) Recommended books and literature:

The textbook will suffice for most purposes, but if students are interested in using other sources as well, they are encouraged to consult with the instructor. Also, the instructor may point out some specific literature for (individual) students to use.

V. Course organization and requirements

Each week there will be two classroom meetings. During these sessions we will:

- review the essential parts of theory
- work on problems to build understanding
- focus on some technical details that turn out the most difficult for the participants

- most weeks will feature an ungraded ‘concept test’, which serves to identify what key concepts are clear to students.

Class attendance is mandatory. If you can’t make it, email the instructor in advance. Repeated absences may lead to the deduction of grades (paragraph 3.3 of the student handbook) As there are few students in the class, it will be easy to make appointments outside regular class hours for extra help on whatever subject.

Homework in a given week is due on Fridays. Please hand it on during our class session. Normally you will get feedback on your work the following week. The assigned problems can be found in the calendar below. On homework that is handed in late, the instructor will generally deduct 10% (from a 100 point scale) for each day the work is late.

For any announcements of the instructor, the course Moodle website functions as the official channel of communication. Please check this website very regularly so you don’t miss important information.

This course is subject to UCR academic rules and procedures. Both students and instructors are required to know and follow these rules and procedures.

VI. Assessment

You will have several opportunities to demonstrate that you have acquired the competencies outlined in the previous section. The nature of the tests and the criteria for assessment are as follows:

Homework		Presentation		Exams	
Set 1	7 %	Project	15%	Exam 1	15 %
Set 2	7 %			Exam 2	15 %
Set 3	7 %			Exam 3	20 %
Set 4	7 %				
Set 5	7 %				
All	**35** %	All	**15** %	All	**50** %

For every test you will receive a grade on a scale from 0 to 100. All these grades will be averaged to determine a final grade on the 0-100 scale. The final letter grade is determined by conversion using the standard UCR table (paragraph 6.3.1 in the student handbook)

<u>Criteria for assessment</u>

Homework assignments

Everybody who wants to acquire proficiency in handling physics must practice a lot. You are expected to hand in all assignments on time. You will receive a grade for every homework set. You can also get credit if you don’t have all the right answers – you probably learn most from your mistakes! In case you can’t (completely) solve an assignment, write down where and why you got stuck. (This enables the instructor to help you.) Depending on how far you got with the assignment and on how well you have formulated your problem, you will receive partial credit. For some problems you will need to use a spreadsheet and/or a computer algebra system.

Exams
The type and difficulty of the exam questions is identical to the homework assignments. An exam will focus on material from the chapters indicated in the course schedule.

Writing Project
You will receive an individual topic related to a problem in physical chemistry. In the project you will analyze how the problem was addressed and (partially) solved. You will write a report on this for a (non-expert) audience. More details will be described in a separate document

VII. Course schedule

Week nr dates	**Topics to be discussed**	**Textbook chapters**	**Assignments and assessment**
1A Aug 27	Dawn of Quantum Theory, Schrodinger Equation	Ch. 1-4	
1B Aug 30	Property of gases	Ch. 16	
2A Sept 3	Postulates and principles of Quantum Mechanics	Ch. 1-4	
2B Sept 6	Bolzmann factor and Partition functions	Ch. 17	
3A Sept 10	Postulates and principles of Quantum Mechanics	Ch. 1-4	
3B Sept 13	Bolzmann factor and Partition functions	Ch. 17	Hand in homework set A
4A Sept 17	Harmonic oscillator	Ch. 5	
4B Sept 20	Partition functions and ideal gases	Ch. 18	
5A Sept 24	Solutions of the Schrodinger equation for Hydrogen, Spherical Harmonics	Ch. 6	Hand in Homework Set B
5B Sept 27	Review Exam 1		
6A Oct 1			Exam 1: Ch.1-5 and Ch. 16-17
6B Oct 4	First Law of Thermodynamics	Ch. 19	
7A Oct 8	Approximation methods, variational method	Ch. 7	
7B Oct 11	First Law of Thermodynamics	Ch. 19	
Oct 14-18	F A L L B R E A K		
8A Oct 22	Approximation methods, variational method	Ch. 7	Upload 1st draft of project to Moodle
8B Oct 25	Entropy and Second Law of Thermodynamics	Ch. 20	

9A Oct 29	Multi-electron atoms	Ch. 8-9	Hand in homework set C
9B Nov 1	No class (Moderation)		
10A Nov 5	Chemical bonding	Ch. 9-10	
10B Nov 8	Entropy and Second Law of Thermodynamics	Ch. 20	Hand in homework set D
11A Nov 12	Review Exam 2		
11B Nov 15			Exam 2: Ch.6-7-8 and Ch. 18-19-20
12A Nov 19	Chemical bonding	Ch. 10	Upload 2nd draft of project to Moodle
12B Nov 22	Helmholtz and Gibbs energies	Ch. 22	
13A Nov 26	Kinetic theory of gases	Ch. 27	
13B Nov 29	Chemical kinetics	Ch. 28-29	Hand-in final version of project
14A Dec 3	Chemical kinetics	Ch. 28-29	
14B Dec 6	Chemical kinetics	Ch. 28-29	Hand in homework set E
15A Dec 10	Review Exam 3		
15B Dec 13			Exam 3: Ch.9-10 and Ch. 22 and Ch. 27-29

VIII. Student learning outcomes

The general learning goals for this course are categorized as follows:

Sessions 1A, 2A, 3A, 4A	**Student Learning Objectives**
McQuarrie and Simon Chapter 1: The Dawn of Quantum Theory	- Explain the need for the Planck constant, and be able to compute it from various data sets - Derive and apply formulas of the Bohr model - Apply particle wave duality and Heisenberg uncertainty principle
McQuarrie and Simon Chapter 2: The Classical Wave Equation	- Solve various wave equations (second order partial differential equations with constant coefficients)
McQuarrie and Simon Chapter 3: The Schrodinger Equation and a Particle in a Box	- Solve SE for particle in a box using boundary conditions - Normalize wave functions and compute probabilities - Compute various expectation values
McQuarrie and Simon Chapter 4: Some Postulates and General Principles of Quantum Mechanics	- Apply postulates of QM to describe various systems - Competently use the mathematics of operators, commutators, eigenvectors/eigenfunctions, eigenvalues - Use general formulation of Heisenberg uncertainty principle
McQuarrie and Simon Chapter 5: The Harmonic Oscillator …	- Construct SE for harmonic oscillator, and use solutions for eigenvalues and eigenfunctions to compute energy levels, expectation values, probabilities

Sessions 1B, 2B, 3B, 4B	**Student Learning Objectives**
McQuarrie and Simon Chapter 16: The Properties of Gas	- Use different gas laws to compute properties of assorted gases - Use experimental data (best-fits) to determine constants in gas laws - Find critical values for parameters - Use vd Waals equation to describe gas and liquid states, phase transition
McQuarrie and Simon Chapter 17: The Bolzmann Factgor and Partition Functions	- Explain use of Boltzmann factor Exp[-E/kT] - Define Partition Function Q and relate to mean energy U=<E> - Relate Partition Function Q to molecular partition function q, understanding when Boltzmann statistics are valid - Determine heath capacity for various systems
McQuarrie and Simon Chapter 18:	- Determine Partition function for ideal monoatomic quantum gas

Partition Functions and Ideal Gasses	

Sessions 5A, 6A, 7A, 8A	Student Learning Objectives
McQuarrie and Simon Chapter 6: The Hydrogen Atom	- Understand definition and usage of spherical coordinates - Understand derivation of spherical harmonics and radial solutions from Schrodinger equation. - Compute probabilities and averages using spherical harmonics and radial solutions
McQuarrie and Simon Chapter 7: Approximation Methods	- Understand basic principles of variational method - Apply variational method to compute ground state energy of various systems. (This requires strong skills in evaluating integrals, possibly using Mathematica) - Understand basic principles of perturbation theory. - Apply perturbation theory to a variety of situations

Sessions 5B, 6B, 7B, 8B	Student Learning Objectives
McQuarrie and Simon Chapter 18: Partition Functions and Ideal Gases	- Determine partition function for oscillator, rotator, .. - Determine most common states at given conditions (like room temperature)
McQuarrie and Simon Chapter 19: The First Law of Thermodynamics	- Explain first law of thermodynamics: $\Delta U = q+w$, using correct signs of q and w. - Compute changes in U and q for various expansions/ compressions of gasses - Explain use of enthalpies, understand different types of enthalpies (formation, combustion, phase transitions, ..) - Compute heat transfer in chemical reactions using enthalpies and Hess Law. - Use both constant and temperature-dependent specific heats correctly

Sessions 9A, 11A, 12A, 12A	Student Learning Objectives
McQuarrie and Simon Chapter 8: Multielectron Atoms	- Define and apply atomic units - Understand concept of electron spin, and apply spin-operator and eigenfunctions - Use spin eigenfunctions to construct complete electron wavefunctions

	- Explain link between Pauli exclusion principle and the notion that electron wavefunctions in atoms must be anti-symmetric - Construct anti-symmetric wavefunctions using Slater determinants.
McQuarrie and Simon Chapter 9: *The Chemical Bond*	- Explain why the stability of a molecular bond is a purely quantum mechanical effect - Evaluate an overlap integral for various situations - Combine wave functions into orbitals

Sessions 9B, 11B, 12B	**Student Learning Objectives**
McQuarrie and Simon Chapter 20: Entropy and the Second Law of Thermodynamics	- Compute entropy changes for various expansions/compressions of gasses - Explain content of Second Law and give examples - For assorted situations determine degeneracy Ω and compute $S = k \ln(\Omega)$ - Compute Entropy S from Partition Function Q
McQuarrie and Simon Chapter 22: Helmholz and Gibbs Energies	- Establish whether a given process will occur spontaneously under specific circumstances - Use relation between equilibrium constant and Gibbs energy for a chemical reaction
McQuarrie and Simon Chapter 27: The First Kinetic Theory of Gases	- Explain how lots of collisions between molecules jointly lead to ideal gas law - Use relationship between temperature and molecule's velocity

Sessions 13B, 14A, 14B	**Student Learning Objectives**
McQuarrie and Simon Chapter 28: Chemical Kinetics I: Rate Laws	
McQuarrie and Simon Chapter 29: Chemical Kinetics II: Reaction Mechanisms	

IX. Appendices [Course specific materials, e.g. guidelines for essays, presentations, etc.]

All additional documents will be placed on Moodle