COURSE DATA

Data Subject	
Code	34193
Name	Physical chemistry I
Cycle	Grade
ECTS Credits	4.5
Academic year	2017 - 2018

Study (s)

Degree	Center	Acad. year	Period
1108 - Degree in Chemistry	Faculty of Chemistry	2	First term

Subject-matter

Degree	Subject-matter	Character
1108 - Degree in Chemistry	7 - Physical chemistry	Obligatory

Coordination

Name	Department
TEJERO TOQUERO, ROBERTO	315 - Physical Chemistry

SUMMARY

Physical Chemistry I is a compulsory subject taught during the first semester of the second year of the Degree in Chemistry. The course is worth a total of 4.5 ECTS credits.

Essentially, this course is intended for students to deepen their understanding of chemistry and physics, which they were taught during the previous year, and to learn how to apply this knowledge to chemical processes. This way, this course serves to establish the necessary grounds for the successful study of future courses on physical chemistry and to provide a framework of reference for all disciplines of the Degree in Chemistry.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

In order to successfully complete the subject, students should have some previous basic knowledge on:

Chemical nomenclature and formulation, both inorganic and organic
Adjustment of chemical reactions
Stoichiometric calculations
Basic knowledge of acid-base reactions, precipitation and redox
Basic knowledge of batteries and the Nernst equation

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

1108 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.
- Show inductive and deductive reasoning ability.
- Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Demonstrate the ability to adapt to new situations.
- Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.
- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them.
- Demonstrate knowledge of the main types of chemical reaction and their main characteristics.

- Demonstrate knowledge of the principles of quantum mechanics and their application to the description of the structure and properties of atoms and molecules.
- Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry.
- Relate the macroscopic properties and the properties of individual atoms and molecules, including macromolecules (natural and synthetic), polymers, colloids and other materials.
- Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.
- Solve qualitative and quantitative problems following previously developed models.
- Recognise and analyse new problems and plan strategies to solve them.
- Evaluate, interpret and synthesise chemical data and information.
- Handle chemicals safely.
- Handle the instrumentation used in the different areas of chemistry.
- Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them.
- Relate theory and experimentation.
- Recognise and evaluate chemical processes in daily life.
- Understand the qualitative and quantitative aspects of chemical problems.
- Develop sustainable and environmentally friendly methods.
- Relate chemistry with other disciplines.
- Students must be able to apply their knowledge to their work or vocation in a professional manner and have acquired the competences required for the preparation and defence of arguments and for problem solving in their field of study.
- Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration.
- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

At the end of the course students should be able to:

- Obtain the order and rate constant of simple and complex chemical reactions from experimental data and use different methods of determination. Use the knowledge acquired in Chemical Informatics.
- Use the rare-limiting step and the steady-state approximations to determine whether a proposed mechanism for a chemical reaction is compatible with the kinetic data available.
- Know some complex reaction mechanisms and understand catalysis.
- Extract information from a phase diagram of a pure substance.
- Use Clapeyron equation to derive an approximate expression for the solid-liquid equation and Clausius-Clapeyron equation (non-condensed phase - condensed phase equation), and use this last expression to deduce the dependence of vapour pressure on temperature.
- Calculate melting and boiling points from thermodynamic quantities and vice versa.
- Calculate the change in melting point with pressure.
- Calculate partial molar quantities.
- Calculate thermodynamic quantities of mixing for ideal solutions.
- Calculate vapour pressure using Raoult and Henry laws.
- Calculate Henry's law constant using vapour pressures of dilute solutions.
- Calculate the increase in the boiling point and the decrease in the freezing point from temperature-composition data.
- Calculate osmotic pressure in ideal dilute solutions.
- Calculate activity coefficients from vapour pressure measurements using the two conventions (symmetrical and asymmetrical).
- Calculate thermodynamic and excess functions for real solutions.
- Calculate activity coefficients of a non-volatile solute based on the solvent’s vapour pressure and on colligative properties, using the Gibbs-Duhem equation.
- Construct and interpret P-x and T-x diagrams of binary solutions.
- Use a temperature-composition diagram to analyse the distillation of a mixture.
- Know the application of Gibbs-Duhem-Margules equation.
- Calculate mean ionic activity coefficients from vapour pressures and colligative properties.
- Know the validity of theoretical expressions to calculate mean ionic activity coefficients (extended or limiting Debye-Hückel law, Davies equation).
- Calculate the equilibrium constant and free enthalpy change from the equilibrium composition.
- Calculate the equilibrium constant from free enthalpy change.
- Calculate the quantities of different substances in a system when it reaches a steady state.
- Predict the movement of a chemical equilibrium when subjected to a change in the equilibrium conditions.
- Calculate the equilibrium constants of non-ideal systems based on free enthalpy change.
- Calculate the equilibrium modalities of electrolyte balance (ionization of acids, slightly soluble salts) by using the Davies equation to estimate the activity coefficients.
- Calculate free enthalpy change of cell reaction relating it to standard potentials.
- Calculate cell standard potentials from the table of standard electrode potential.
- Calculate the standard potential of a reversible galvanic cell using the Nernst equation.
- Calculate the thermodynamic properties of the reaction from the dependence of standard potential on temperature.
- Calculate equilibrium constants from standard potential data.

Calculate activity coefficients from the potential of electrodes of a cell by using the electrochemical equilibrium condition at the electrodes.

DESCRIPTION OF CONTENTS

1. Formal kinetics

Introduction. Complex reactions: reversible reactions, competitive reactions, consecutive reactions. Reaction mechanisms. Molecularity. Limiting-step approximation. Steady-state approximation. Influence of temperature on reaction rate. Variation of rate constant with temperature. Catalysis.

2. Open systems and changes in composition. Partial molar properties and chemical potential

Introduction. Properties of the Gibbs function (free energy). Dependence of Gibbs function on temperature. Dependence of Gibbs function on pressure. Thermodynamic description of mixtures. Partial molar quantities (properties). Partial molar Gibbs function or chemical potential. Material balance. Gibbs-Duhem equation. Relation between partial molar quantities. Thermodynamic functions of mixing. Chemical potential of ideal gas and ideal gas mixtures.

3. Simple applications of material equilibrium

Changes of state of pure substances and thermodynamics of ideal solutions. The concepts of phase and component. Phase rule. Phase diagrams of one-component systems. Examples. Phase equilibrium. Stability of the phases, curves of chemical potential versus T. Dependence curves of chemical potential versus T with pressure. Clapeyron equation. Variation of equilibrium pressure with temperature. Solid-liquid equilibrium. Equilibrium liquid/gas. Equilibrium solid/gas. Chemical potential of liquids (solutions). Ideal solutions: Raoult's law. Thermodynamic properties of solutions. Dilute ideal solutions: Henry's law. Thermodynamic properties.

4. Colligative properties. Activity coefficients

Introduction. Colligative properties. The common feature of colligative properties. Lowering the vapour pressure. Boiling point elevation. Freezing point depression. Osmotic pressure. Real solutions: activities and activity coefficients. The activity of the solvent. Symmetric Convention (I). The activity of the solute. Asymmetric Convention (II). Conventions, scales and reference states. Determination of activities and activity coefficients. Determination of activity coefficients from measurements of vapour pressure. Determination of activity coefficients from colligative properties. Gibbs-Duhem-Margules equation. Excess thermodynamic functions.

5. Phase equilibria of binary systems

Introduction. Phase diagrams for binary solutions. Vapour pressure-composition diagrams. Temperature-composition diagrams. Representation of the distillation. Distillation of real solutions: azeotropes. Distillation of immiscible liquids.

6. Electrolyte solutions

Electrolyte solutions. Introduction. Electrolyte solutions. Chemical potential of a composite electrolyte. Chemical potential of an electrolyte. Determination of activity coefficients of electrolytes. Practical osmotic coefficient of the solvent. Determination of the ionic activity coefficient from measurements of colligative properties. Empirical behaviour of solutions of electrolytes. Debye-Hückel model for electrolyte solutions.

7. Chemical equilibrium

Introduction. Spontaneous chemical reactions. The minimum Gibbs function. Thermodynamic condition for chemical equilibrium. Affinity. Chemical balance in a mixture of ideal gases. Equilibrium constants based on concentrations and mole fractions. Variation of equilibrium constant with temperature and pressure. Le Chateliers principle. Chemical equilibria in real gases. Fugacity of a real gas. Chemical equilibrium in ideal non-electrolyte solutions. Actual chemical balance in non-electrolyte solutions. Heterogeneous equilibrium. Ionic equilibria (solutions of electrolytes). Ionization equilibria of weak acids. Solubility equilibria.

8. Electrochemical equilibrium

Electrochemical equilibrium. Electrode potential. Electrochemical potential properties. Types of electrodes. Electromotive force. Thermodynamics of a battery. Measurement of thermodynamic quantities from the potential difference between electrodes of a battery. Liquid junction potential. Applications of EMF measurements: activity coefficient, pK, solubility product, and prediction of the spontaneity of redox reactions and metal corrosion.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	38,00	100
Tutorials	7,00	100
Study and independent work	30,00	0
Preparation of evaluation activities	16,00	0
Preparing lectures	6,50	0
Preparation of practical classes and problem	15,00	0
TOTAL	**112,50**	

TEACHING METHODOLOGY

The course is delivered in three areas: theoretical and practical classes, conferences and/or seminars, and other activities during non-classroom hours. Theoretical and practical classes will provide an overview of the topic and will focus on its key concepts. Recommended resources for further in-depth study of the subject will also be provided.

In some sessions the lecturer will explain a number of typical problems through which students can learn to identify the essential elements of the approach and to solve the problems proposed. In other sessions, however, the students will play a leading role, as it will be them who will have to deal with similar or more complex problems. Students will be allocated into groups and the lecturer will guide and help them.

As for tutorials, there will be 7 sessions throughout the semester. In them, the lecturer will advise students on all the elements of the learning process, both as regards global approaches and specific issues. Also, students will be given a list of questions and additional problems that will serve to reinforce their knowledge and to practise each of the matters covered in the classroom sessions. The student must solve and submit all the problems and questions that the lecturer requests.

As for programmed conferences where current topics will be tackled, at the end of the session, the students will answer a test with questions related to the content of the talk.

EVALUATION

The assessment of learning will take account of three different items:

1. Ongoing assessment of progress and activities carried out throughout the course (largely based on questions and problems given to students and on the work done in the tutorial sessions) will account for 20% of the final grade. Attendance to the interdisciplinary conferences will be evaluated through a test, whose mark will be added as a 5% to the qualification of the ongoing assessment.
2. An additional 10% will be obtained through the preparation and presentation of one or more essays.
3. A final exam will contribute 70% of the final mark. Exams will consist of a first part of objective questions covering basic knowledge and a second part containing general problems.

Moreover, each of the items considered in the assessment require a minimum mark of 40%.

In exceptional duly justified cases, the student may request, in writing at the beginning of the course, to be assessed only through a final exam.

For the second examination sitting the same criteria apply.

REFERENCES

Basic

- Engel,T y Reid, P. Química Física. Pearson Addison Wesley, 2006. ISBN 9788478290772
- Atkins, P. y De Paula, J. Química Física. 8ª ed. Editorial Médica Panamericana, 2008. ISBN 9789500612487
- Levine, I. N. Fisicoquímica. 5ªed. MacGraw-Hill, 2004. ISBN 9788448137861 (v. 1) ISBN 9788448137878 (v. 2)