COURSE DATA

Data Subject	
Code	34193
Name	Physical Chemistry I
Cycle	Grade
ECTS Credits	4.5
Academic year	2021 - 2022

Study (s)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Faculty of Chemistry	2	Second term

Subject-matter

Degree	Subject-matter	Character
1110 - Degree in Chemistry	7 - Physical Chemistry	Obligatory

Coordination

Name	Department
SANCHEZ DE MERAS, ALFREDO	315 - Physical Chemistry

SUMMARY

Physical Chemistry I is an obligatory subject taught in the second half of the second year of the grade studies in Chemistry. The course has a total of 4.5 ECTS credits.

This course aims, essentially, to deepen the knowledge of Chemistry and Physics that the students should have obtained in the previous year and to learn how to apply them to chemical processes. In this way, this course establishes the necessary grounds for the successful study of the future courses of Physical Chemistry as well as a support of reference for all disciplines of the Chemistry grade.

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 achieve success in the subject, the students should have basic knowledge on:

Nomenclature and formulation chemistry, 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.

OUTCOMES

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

The previous section includes the competences contained in the document VERIFICA. This subject addresses part of the learning results of the matter PHYSICAL CHEMISTRY I that allow to acquire specific knowledge of chemistry, cognitive skills and general skills recommended by the EUROPEAN CHEMISTRY THEMATIC NETWORK (ECTN) for the Chemistry Eurobachelor® Label. The following table lists the learning outcomes acquired in the subject PHYSICAL CHEMISTRY I related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject PHYSICAL CHEMISTRY I that contemplate the learning outcomes EUROBACHELOR®
The characteristics of the different states of matter and the theories used to describe them.	Demonstrate knowledge of the characteristics and behaviour of the different states of matter and the theories used to describe them..(CE3).
The principles of thermodynamics and their applications to chemistry	Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry..(CE6).
The kinetics of chemical change, including catalysis; the mechanistic interpretation of chemical reactions	Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry..(CE6).

COMPETENCES AND COGNITIVE SKILLS	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject PHYSICAL CHEMISTRY I that contemplate the learning outcomes EUROBACHELOR®
Ability to demonstrate knowledge and	Demonstrate knowledge and understanding of

understanding of the facts, concepts, principles and fundamental theories related to the topics mentioned above.	essential facts, concepts, principles and theories related to the areas of chemistry..(CE13).
Ability to apply this knowledge and understanding to the solution of common qualitative and quantitative problems.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Competences to present and argue scientific issues orally and in writing to a specialized audience.	Relate chemistry with other disciplines.(CE26). Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate. (CG6). Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences..(CB4).
Ability to calculate and process data, related to information and chemistry data.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15).

COMPETENCES AND COGNITIVE SKILLS RELATED TO THE PRACTICE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject PHYSICAL CHEMISTRY I that contemplate the learning outcomes EUROBACHELOR®

GENERAL COMPETENCES	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject PHYSICAL CHEMISTRY I that contemplate the learning outcomes EUROBACHELOR®
Ability to apply practical knowledge to solve problems related to qualitative and quantitative information.	Solve problems effectively..(CG4). Solve qualitative and quantitative problems following previously developed models..(CE14). Relate theory and experimentation..(CE22). Recognise and evaluate chemical processes in daily life..(CE23). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Calculation and arithmetic capabilities, including aspects such as analysis error, estimates of orders of magnitude, and correct use of the units.	Develop capacity for analysis, synthesis and critical thinking..(CG1). Show inductive and deductive reasoning ability..(CG2). Solve problems effectively..CG4).
Ability to adapt to new situations and make decisions.	Demonstrate the ability to adapt to new situations..(CG9). Recognise and analyse new

	problems and plan strategies to solve them..(CE15). 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..(CB3).
Planning and time management skills.	Develop capacity for analysis, synthesis and critical thinking.(CG1). Solve problems effectively..CG4).
Study skills necessary for professional development. These will include the ability to work autonomously.	Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5). Learn autonomously.(CG8). Demonstrate the ability to adapt to new situations..(CG9). Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.(CB5).
Ethical commitment to the European Code of Conduct: http://ec.europa.eu/research/participants/data/ref/h2020/other/hi/h2020-ethics_code-of-conduct_en.pdf	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.(CB3).

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

- Get the order and rate constant of simple and complex chemical reactions from experimental data and use different methods of determination. Using the knowledge acquired in Computer Applications.
- Use approximations of the limiting step and the steady state to determine whether a proposed mechanism for a chemical reaction.
- Know some complex reaction mechanisms and understanding the catalysis.
- Extract information from a phase diagram of a pure substance.
- Use Clapeyron’s equation to derive an approximate expression for the solid-liquid equation and Clausius-Clapeyron equation (equation no condensed-phase condensed phase), and use this last expression to deduce the dependence of vapor 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 the vapour pressure using Raoult and Henry laws.
- Calculate Henry's law constant using vapour pressures of dilute solutions.
- Calculate the boiling point elevation and freezing point depression data from temperature-composition.
- Calculate the osmotic pressure in ideal dilute solutions.
- Calculate the activity coefficients from vapour pressure measurements using the two conventions (symmetrical and asymmetrical).
- Calculate excess thermodynamic functions for real solutions
- Calculate the activity coefficients of a non-volatile solute data from the solvent vapour pressure and 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 analyze the distillation of a mixture
- Know the application of Gibbs-Duhem-Margules.
- Calculate mean ionic activity coefficients from vapour pressures and colligative properties.
- Know the validity of the theoretical expressions to calculate mean ionic activity coefficients (extended and limiting laws of Debye-Huckel, 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 steady state.
- Predict the movement of a chemical equilibrium when subjected to a change in the equilibrium conditions.
- Calculate equilibrium constants of non-ideal systems based on free enthalpy change.
- Calculate the equilibrium molalities of electrolyte balance (ionization of acids, slightly soluble salts) using the Davies equation to estimate the activity coefficients.
- Calculate the free enthalpy change of a 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 Nernst equation.
- Calculate thermodynamic properties of a 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 the Gibbs function with the temperature. Dependence of the Gibbs function with the pressure. Thermodynamic description of mixtures. Quantities (properties) partial molar. 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. 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.

4. Colligative properties. Activity coefficients

Chemical potential of liquids (solutions). Ideal solutions, Raoult's law. Thermodynamic properties of solutions. Dilute ideal solutions: Henry's law. Thermodynamic properties. Colligative properties. The common feature of colligative properties. Lowering of the vapor 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 vapor pressure. Determination of activity coefficients from colligative properties. Gibbs-Duhem-Margules. Excess thermodynamic functions.

5. Phase equilibria of binary systems

Introduction. Phase diagrams for binary solutions. Diagrams vapor pressure-composition. Temperature-composition diagrams. Representation of the distillation. Distillation of real solutions: azeotrope. 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. The practical osmotic coefficient of solvent. Determination of ionic activity coefficient from measurements of colligative properties. Empirical behavior 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 stack. Measurement of thermodynamic quantities from the potential difference between electrodes of a battery. Liquid junction potential. Applications of the FEM as d: activity coefficient, pK, solubility product, and predicting 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

Development of the course is structured around three areas: theoretical and practical classes, seminars and other activities in the non-attending hours. Theoretical and practical classes will give an overview on the topic and will have an impact on those key concepts for understanding it. It will also provide more recommended resources for further preparation of the subject in depth.

In some sessions the student will explain a number of problems-type through which learn to identify the essential elements of the approach and solve the problems posed by this issue. In other sessions, however, ownership will pass completely into the hands of the student, as it will be he who will face similar problems and more complex. Students are allocated to groups and the teacher will guide them and help.

With respect to tutorials, there will be 7 sessions in the semester. In them, the teacher will guide students on all elements of the learning process, both in regard to global approaches as to specific issues. Also, students will receive them a list of questions and additional problems that will reinforce their knowledge and exercise in each of the matters covered in the class sessions. The student must submit unresolved issues and questions that the Professor indicates.

EVALUATION

The assessment of learning will take place in two different ways:

1. Ongoing assessment of progress and activities throughout the course. The grade in this section will represent 30% of the final grade.

2. A final exam that will contribute to the final grade by 70%. The exam can include questions (either theoretical or numerical) and problems. A minimal grade of 4.0 is required in order the ongoing assessment to be considered for the global grade.

For the second evaluation, the same criteria exposed above will be applied

REFERENCES

Basic

- ENGEL, T., REID, P. Química Física. Pearson Addison Wesley, 2006. ISBN 9788478290772
- ATKINS, P., 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)

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

Contents

1.- The contents initially indicated in the teaching guide are maintained.

Workload and temporary teaching planning

Regarding the workload:

1.- The different activities described in the Teaching Guide are maintained with the intended dedication.

Regarding the temporary teaching planning:

2.- The material to follow the theory/tutoring/classroom-seminar classes allows to continue the temporary teaching planning both in days and schedule, whether the teaching is face-to-face in the classroom or not, although in some of the activities the student has the freedom to follow the non-face-to-face sessions according to his own planning.

Teaching Methodology

Theory subjects:

Situation of minimal attendance: In theory classes and tutorials the occupation will be, at most, 30% of their usual occupation. Teaching will be online. Students who have a laboratory session before or after theory classes, and the time to travel is longer than the time established in the schedules, will be able to follow the class in person in the classroom assigned in the schedules. When there are students in this situation, classes will be taught by synchronous videoconference in the group classroom.

Maximum face-to-face situation: In theory classes and tutorials, the occupation will respect the sanitary restrictions that limit the capacity of the classrooms. Depending on the capacity of the classroom and the number of students enrolled, it may be necessary that part of the students have to follow the classes synchronously. If this situation arises, the students will attend the group classroom in weekly rotating shifts (preferably in alphabetical order), so as to ensure that the percentage of attendance of all the students enrolled in the subject is the same.

Confinement situation: If for health reasons it is not possible to continue with hybrid teaching, totally or partially affecting the classes of the subject, these will be replaced by synchronous non-face-to-face sessions following the established schedules and using the virtual classroom tools.

The methodology used for non-face-to-face classes shall be:

1. Synchronously using virtual classroom tools (preferably Teams)

2. Asynchronously using presentations with audio narration or other virtual classroom tools

3. Resolution of exercises and questionnaires

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In all subjects

If there is a closure of the facilities for health reasons that totally or partially affects the classes of the course, they will be replaced by non-face-to-face sessions following the established schedules and using the tools of the virtual classroom.

In the case of students confined to home due to COVID, they will be ensured on-line teaching through Teams.

Evaluation

The possibility of exam-only evaluation is eliminated (except very well justified cases).

If there is a closure of the facilities for health reasons affecting the development of any face-to-face evaluable activity of the subject, it will be replaced by a test of a similar nature that will be carried out in virtual mode using the computer tools licensed by the University of Valencia. The contribution of each evaluable activity to the final grade of the subject will remain unchanged, as set out in this guide.

References

2.- The literature recommended in the Teaching Guide is maintained since it is accessible, and it is complemented by notes, slides and problems uploaded to the Virtual Classroom as material of the course.