Universidad Zaragoza

Year : 2019/20

27207 - Physical Chemistry I

Syllabus Information

Academic Year: 2019/20
Subject: 27207 - Physical Chemistry I
Faculty / School: 100 -

Degree: 452 - Degree in Chemistry

ECTS: 10.0
Year: 2
Semester: Annual
Subject Type: Compulsory
Module: ---

1.General information

1.1.Aims of the course

1.2.Context and importance of this course in the degree

1.3.Recommendations to take this course

2.Learning goals

2.1.Competences

2.2.Learning goals

2.3.Importance of learning goals

3.Assessment (1st and 2nd call)

3.1.Assessment tasks (description of tasks, marking system and assessment criteria)

4.Methodology, learning tasks, syllabus and resources

4.1.Methodological overview

The methodology followed in this course is oriented towards achievement of the learning objectives. It is strongly related to understanding and reasoning processes. A wide range of teaching and learning tasks are implemented, such as theoretical sessions, problem-solving sessions, seminars, course works and tutorials.

Students are expected to participate actively in the class throughout the course.

Classroom materials will be available via Moodle. These include a repository of the lecture notes used in class, the course syllabus, as well as other learning resources such as problem and question to solve or answer, and online support material.

Further information regarding the course will be provided on the first day of class.

4.2.Learning tasks

The course includes 10ECTS organized according to:

- Formative activity 1: Interactive lecture classes on Physical Chemistry (6 ECTS)
    - Physical Chemistry (Thermodynamic of Chemical Systems): 42 hours (22 theory + 20 problems).
    - Physical Chemistry (Electrolytes and Thermodynamic of Electrochemical Systems): 26 hours (17 theory + 9 problems).

- Physical Chemistry (The Kinetic of Chemical Reactions): 32 hours (21 theory + 11 problems).

- Formative activity 2: Problems and case?based solving sessions and seminars (4ECTS). A series of problems will be available for the students to work in advance. The classes will take place in small groups; some of the problems will be solved by the teacher, some by the students, and some worked out in groups. In this formative activity is essential the participation of the students.

4.3.Syllabus

The course will address the following topics:

Section 1. Thermodynamic of Chemical Systems: 42 hours (22 theory + 20 problems)

- Topic 1. Introduction and fundamental concepts, including mathematical tools to handle state functions. Real gases. Thermometry.
- Topic 2. The Principles of Thermodynamics. The First Law. Calculation of thermodynamic properties of ideal gases. Enthalpy of reaction and its dependence with temperature. Reactions in adiabatic conditions. The Second Law: Calculation of Entropy changes in closed systems including cyclic, isothermal, isobaric, isochoric, adiabatic, reversible and irreversible processes of ideal gases. Ideal gases mixing. Entropy and spontaneous processes or equilibrium. Entropy: physical interpretation. Joule and Joule-Thompson effects. The Third Law.
- Topic 3. The Gibbs and Helmholtz functions. Equilibrium criterion. Thermodynamic relationships for closed systems in equilibrium. The Maxwell equations. The Gibbs-Helmholtz equations. Thermodynamic functions and their dependence with p, V and T. Calculation of changes in thermodynamic functions over a range of temperature and pressure.
- Topic 4. Multicomponent systems. Partial molar quantities. The chemical potential. The Gibbs-Duhem equation. General criterion of equilibrium in closed systems. Phase equilibrium of pure substances. The phase rule. The Clapeyron equation. The chemical potential of pure substances. Behaviour of real gases. Mixtures of real gases.
- Topic 5. Definition of the ideal solution. Raoult and Henry laws. The ideal solubility of gases in liquids. The ideal solubility of solids in liquids. Colligative properties. Relative lowering of vapour pressure. Boiling point elevation. Freezing point depression. The osmotic pressure of an ideal solution. Colligative properties of electrolytic solutions. Partition coefficient.
- Topic 6. Definition of non-ideal solution. Chemical potential, activity, and vapour pressure of each substance in non-ideal solutions. Determination of activity coefficients. Conventions for activity coefficients. The use of molality and concentration scales. Electrolytic solutions. Mean activity coefficient.
- Topic 7. Phase equilibrium in multicomponent systems. Vapour-liquid equilibrium in ideal and non-ideal solutions. Lever rule. Azeotropic mixtures. Simple and full distillation. Partially miscible systems. Non-miscible systems.
- Topic 8. Chemical equilibrium. The equilibrium constant. Reaction equilibrium in ideal and real gases. Reaction equilibrium in solutions. Temperature and pressure dependence of the equilibrium constant. Le Chatelier's principle.

Section 2. Electrolytes and Thermodynamic of Electrochemical Systems: 26 hours (17 theory + 9 problems).

- Topic 9. Electrolytes: Descriptive introduction of the Debye-Hückel limiting law. Variation of the activity coefficient with the electrolyte concentration in aqueous solution. Electric current; Ohm's Law in metals and ionic solutions. Conductivity measurements of an electrolyte solution. Kohlrausch Law of independent migration of ions. Molar conductivity. Effect of concentration on molar conductivity. Asymmetry effect and electrophoretic effect. Ion transport number. Determination of ion transport numbers by Hittorf method and moving-boundary method.
- Topic 10. Electrochemistry: Electrochemical systems. Thermodynamics of electrochemical systems, the electrochemical potential. Galvanic cells. Electromotive force. Daniell cell. Electromotive force measurements on cells. Types of reversible electrodes. Galvanic Cells and the Nernst Equation. Liquid junction potential. Standard electrode potential. Thermodynamic properties determined by the measurement of the electromotive force: equilibrium constant, activity coefficient, potentiometric titration. Concentration cells with and without transport. Batteries. Fuel cells.

Section 3. The Kinetic of Chemical Reactions: 32 hours (21 theory + 11 problems).

- Topic 11. Kinetics of chemical reactions: Introduction and basic concepts. Measurements of reaction rates. The rates of reactions, order of reactions. Integration of rate laws: irreversible, reversible, consecutive and competing reactions, reactions approaching equilibrium. Determination of the rate law.
- Topic 12. Mechanisms of chemical reactions: the rate-limiting-step approximation and the steady-state approximation. From rate law to mechanism. Relation between rate constants for the forward and backward reactions.
- Topic 13. The temperature dependence of reaction constant: Arrhenius equation and activation energy.
- Topic 14. Unimolecular reactions: Lindemann mechanism. Trimolecular reactions.
- Topic 15. Chain reactions. Kinetics of formation of HBr from H2 and Br2. Organic decompositions; Rice-Herzfeld

mechanism. Free radical polymerization kinetics. Branched chain reactions.

- Topic 16. Catalysis. Homogeneous catalysis in gas phase: catalytic destruction of ozone in the Earth's stratosphere. Homogeneous catalysis in liquid phase: Acid-base catalysis. Enzyme catalysis. Michaelis-Menten mechanism. Inhibition in enzyme catalysis: reversible and irreversible.

4.4.Course planning and calendar

For further details concerning the timetable, classroom and further information regarding this course please refer to the ?Facultad de Ciencias " website (http://ciencias.unizar.es).

4.5.Bibliography and recommended resources

http://biblos.unizar.es/br/br_citas.php?codigo=27207&year=2019