

Anno Accademico 2019/2020

PHYSICAL CHEMISTRY AND LABORATORY - 1

Enrollment year

2018/2019

Academic year

2019/2020

Regulations

DM270

Academic discipline

CHIM/02 (PHYSICAL CHEMISTRY)

Department

DEPARTMENT OF CHEMESTRY

Course

CHEMISTRY

Curriculum

PERCORSO COMUNE

Year of study

2°

Period

1st semester (01/10/2019 - 17/01/2020)

ECTS

9

Lesson hours

72 lesson hours

Language

Italian

Activity type

WRITTEN AND ORAL TEST

Teacher

BERBENNI VITTORIO (titolare) - 6 ECTS CAPSONI DORETTA - 3 ECTS

Prerequisites

For what concerns General Chemistry, reference will be made to 1) Chemical Reactions and their stoichiometric balance . This will be useful to introduce the thermal balane of chemical reactions (Hess Law) 2) Chemical equilibrium. Law of mass action. This will serve as a basis for the introduce the chemical potential and the activity. This fine tunes the law of mass action and allow also the consideration of chemical equilibria in non ideal and/or inhomogeneous equilibrium. 3) Phase diagrams of pure compounds (e.g. water and carbon dioxide) . Diese knowledge will be extended by adding the variable composition so as that the students shoulbe capable of interpreting the two-components phase diagrams.

For what concerns Physics the general concepts (first of all the electromagnetic spectrum) are needed while for what concerns mathematics the students will be requested to be able to execute derivative and integral of elementary functions.

Learning outcomes

The three principles of thermodynamics. The main thermodynamic functions: internal energy, enthalpy, entropy, free energy of Gibbs and Helmoltz. The chemical and the phase equilibrium. The thermodynamic properties of mixtures.

The quantum mechanics: the Schroedinger equation. The operators. The solutions of the Schroedinger equation for the hydrogen athom.

Course contents

The first principle of thermodynamics: heat and work. The thermodynamic properties internal energy (U) and enthalpy (H). The relationship between U und H. Thermochemistry: the formation enthalpy. What is it, how can it be determined, what is its use. The integral enthalpy of dissolution: the formation enthalpy of ions. The thermodynamic cycle of Born-Haber. Enthalpy of chemical reaction and its dependence on the temperature. Relationship between the enthalpy of formation and the bond energy: some examples. Calorimetry: classification of calorimeters based on operation mode and on working principle.

The second principle of thermodynamics: the function entropy and its thermodynamic and statistic definition. Entropy and spontaneous processes. Entropy changes with pressure and temperature. The transition entropy. The third principle of thermodynamics: the calculation of the absolute entropy of a substance as a function of temperature. The functions G and A: physical meaning. The differential of the functions U, H, S, G, A. The Maxwell's relationships. The relationships between Cp and Cv.

Phase equilibrium: the Gibbs Theorem. Phase equilibrium in one-component system. The phase rule. Phase equilibrium in two-component systems: the liquid-vapor and the solid-liquid equilibria. Phase diagrams. The thermodynamic properties of mixtures: the partial molar volume and the chemical potential. Ideal and real mixtures: the activity and the activity coefficient. The chemical equilibrium: the equilibrium constant and its dependence on pressure and temperature. Calculation of the equilibrium constant.

The unanswered questions of classical physics and the quantum mechanics. The Schroedinger equation. The Wave function and the Born interpretation of the wave function. The operators and the Heisemberg principle. Applications: the particle in a box, the harmonic oscillator, the rigid rotor and the particle on a spherical surface. Structure and spectra of the hydrogen atoms. The quantic numbers.

Teaching methods

All the topics will be presented in the lessons. At the end of every group of lesson (between 2 and 4 lessons) problems on the topics just presented will be solved through a discussion with the students. This should ease the understanding by the students of the presented topics

Reccomended or required readings

Peter Atkins- Julio de Paula "Chimica Fisica" (V italian edition translated from the IX english edition) Zanichelli.

Some written material and excercises with solutions provided by the teacher per e-mail.

Assessment methods

Written and Oral Exams. In the written part the students will have to solve exercises on the three principles of thermodynamics (enthalpies of reactions and entripies of reactions with the aim to calculate the

equilibrium constants of chemical reactions.

Furthermore the students shall also be capable to solve exercises on partial molar volume, mixture properties (law of Raoult and Henry) and colligative properties so as to be able to calculate activities of the components of these systems. Finally the will have to show how a two components solid-liquid diagrams will be interpretated.

The oral part will be devoted to the discussion of errors made from the students in the written part . Finally a discussion on simply topics of quantomechanics will complete the exam.

Further information

Nothing special

Sustainable development goals - Agenda 2030

\$lbl legenda sviluppo sostenibile