UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO

dipartimento di farmacia-scienze del farmaco

General information		
Academic subject	PHYSICAL CHEMISTRY	
Degree course	Pharmaceutical Chemistry and Technology LM-13	
Year of study	Second year	
European Credit Transfer and Accumulation System (ECTS)	8	
Language	Italian	
Academic Year	2022-2023	
Academic calendar (starting and ending date)	First semester (20 September 2021 - 21 January 2022)	
Attendance	mandatory attendance	

Professor/ Lecturer	
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Virtual headquarters	Microsoft Teams platform, course code *yp8dfcv*
Tutoring (time and day)	By appointment, to be agreed via e-mail

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Syllabus	
Learning Objectives	The course aims to provide students with the fundamentals of thermodynamics, chemical kinetics and molecular spectroscopy with the aim of transmitting the knowledge and tools necessary to face and solve problems inherent to physical chemistry.
Course prerequisites	Basic knowledge of General and Inorganic Chemistry, Mathematics and Physics
Contents	**1.0 The properties of gases.** 1.1 Equation of state of ideal gases. 1. 2 Kinetic theory of gases: 1.3 Real gases. Virial equation of state. Van der Waals law. **2.0 Chemical thermodynamics**. 2.1 Introduction. Definition of system, environment, variables or thermodynamic functions. States of equilibrium and thermodynamic transformations. Heat and Work. Calorimetry. 2.2 The first principle. Internal energy. Thermal capacity and specific heat. 2.3 Enthalpy. Enthalpy of physical, atomic and molecular transformations. Thermochemistry. Law of Hess. Standard enthalpy of formation. Variation of enthalpy with temperature: Kirchhoff's law. 2.4 Second principle. Statements. Spontaneous transformations. Reversibility and irreversibility. 2.5 Entropy. Thermodynamic definition. Clausius inequality. Adiabatic transformations. Thermodynamic cycles. Carnot's theorem and cycle. Refrigerant cycles. Entropy of a state transition. Entropy variation with temperature. Absolute entropy. 2.6 Third principle. Nernst's theorem. Boltzmann relation. 2.7 Helmholtz energy and Gibbs energy. Maximum work function. Free energy of reaction. Fundamental equation of thermodynamics. Maxwell relations. Thermodynamic equation of state. Variation of Gibbs energy with pressure and temperature. Gibbs-Helmholtz equation. Fugacity and activity. Partial molar sizes. Chemical potential. Thermodynamic criterion of equilibrium. Clapeyron equation. Gibbs energy of mixing. Reaction

	quotient and equilibrium constant. Le Chatelier's principle. Van't Hoff equation. **3.0 Properties of solutions.** 3.1 Colligative Properties. 3.2 Solubility. 3.3 Repartition of a solute among immiscible liquids. **4.0 Phase equilibria**. 4.1 State diagrams of mixtures. Two-component systems and temperature-composition diagrams. Solid-liquid systems: diagrams with eutectic; solid solutions. Liquid-liquid state diagrams for partially miscible two-component systems. Liquid-vapor state diagrams for mixtures of volatile liquids: simple and fractional distillation; azeotropes; distillation of immiscible liquids. **5.0 Disperse systems: Colloids and surfactants.** 5.1 Cohesion forces. Molecular interactions. Surface tension. 5.2 Colloids: definition and properties. Tyndall effect. Colloids: classification. Coagulation and flocculation. 5.4 Surfactants: classification. Micelles and liposomes. Hydrophobic interaction. Biological membranes. Liquid crystals. **6.0 Chemical kinetics.** 6.1 Reaction rates, rate constants and kinetic laws. Order of reaction. Kinetic laws in integrated form. Reactions of order 0, of the first, second and n order. Pseudo-order. Half-life. Molecularity of reactions. Elementary and non-elementary reactions. Kinetics of equilibrium reactions, of consecutive and competitive reactions. 6.2 Dependence of the reaction rate on the temperature. Arrhenius equation. Collision theory. Activated complex and transition state theory. Catalysis. Homogeneous and heterogeneous catalysts. Enzymes and enzymatic catalysis. **7.0 Quantum theory** 7.1 Failures of classical mechanics. Black body radiation. Low temperature heat capacity: Debye relation. Photoelectric effect. Wave-particle dualism: De Broglie relation. Wave functions. Schrödinger equation. Interpretation of Born. Heisenberg's uncertainty principle. **8.0 Atomic and molecular structure.** 8.1 Spectra and structure of hydrogen atoms. Quantum numbers. Wave functions and orbitals. 8.2 The spin. Selection rules. Pauli exclusion principle. Hund's rule. 8.3 Chemical bond. Valence bond theory. Hybrid orbitals. Resonance. 8.4 Theory of molecular orbitals. LCAO method **9.0 Molecular spectroscopy.** 9.1 General aspects. Rotational, vibrational and electronic spectroscopy. Fluorescence and phosphorescence. Principles of Nuclear Magnetic Resonance.
Books and bibliography	P.W. Atkins, J. De Paula. Elements of Physical Chemistry, Zanichelli, Bologna P.W. Atkins Physical Chemistry (third Italian edition) Zanichelli
Additional materials	Publisher's website

Work schedule	

Total	Lectures	Hands on (Laboratory, working groups, seminars, field trips)	Out-of-class study hours/ Self-study hours
Hours			
200	70	10	120
ECTS			
8	7	1	

Teaching strategy	The course includes lectures with the support of PowerPoint presentations (available on teams) and classroom exercises
Expected learning outcomes	
Knowledge and understanding on:	Knowledge and understanding of the principles of the thermodynamics of spectroscopy and of chemical kinetics
Applying knowledge and understanding on:	Acquisition of methodological procedures for applications of thermodynamics, spectroscopy and chemical kinetics for qualitative, quantitative, structural and kinetic determinations
Soft skills	• *Making informed judgments and choices* Acquisition of autonomy in the evaluation and interpretation of experimental data and in setting the strategies for applying the concepts studied in the thermodynamic, spectroscopic and kinetic fields • *Communicating knowledge and understanding* Ability to communicate in written and oral form, in Italian and English, also with the use of multimedia systems. • *Capacities to continue learning* Ability to easily retrieve information from literature, databases and the internet.

Assessment and feedback	
Methods of assessment	Written and oral exam on all the topics of the program.
Evaluation criteria	• *Knowledge and understanding* Students must demonstrate that they have acquired the fundamental concepts of thermodynamics, chemical kinetics and spectroscopy to achieve the skills necessary for the study of the disciplines included in the degree course. • *Applying knowledge and understanding* Students must be able to apply the chemical-physical knowledge in the solution of the proposed exercises. • *Autonomy of judgment* Students will have to demonstrate that they have mastered the basic physico-chemical principles acquired • *Communication skills* Students must be able to express themselves in written and oral form, in a clear and rigorous way. • *Capacities to continue learning* Students must demonstrate that they have critically acquired the fundamental notions and that they are able to identify interconnections and applications of the concepts acquired in real contexts.
Criteria for assessment and attribution of the final mark	The exam includes a written and an oral test. Students will be able to access the oral exam only if they pass the written exam Both tests contribute to determining the final mark. In addition to ascertaining the acquisition of notions, the autonomy of judgment and the ability to argue and explain is evaluated.

	The final mark is awarded out of thirty. The exam is considered passed when the mark is greater than or equal to 18.
Additional information	