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
ECTS credits	8
Compulsory attendance	Yes
Language	Italian
Academic year	2020-2021

Subject teacher	Name Surname	Role
	CATUCCI LUCIA	Associate Professor
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ECTS credits details	Area	SSD	CFU/ETCS
Basic teaching activities	Chemistry (03-A2) Training activities related - integrative	CHIM/02	8

Class schedule	
Period	First semester
Year	Second year
Type of class	Lectures (7 CFU / lessons + 1 CFU / Exercises)

Time management	
Hours	200
In-class study hours	80
Out-of-class study hours	120

Academic calendar	
Class begins	5 October 2020
Class ends	22 January 2021

Syllabus	
Prerequisites/requirements	Basic knowledge of General and Inorganic Chemistry, Mathematics and Physics
Expected learning outcomes	*Knowledge and understanding on:* Acquisition of the fundamental aspects of thermodynamics, chemical kinetics and spectroscopy. *Applying knowledge and understanding* on: Ability to apply the acquired knowledge for the formulation of strategies for solving problems inherent the areas covered by the degree program. *Making informed judgments and choices:* Ability to master the chemical-physical principles acquired to apply them in the disciplines envisaged by the degree course.

	Communicating knowledge and understanding Ability to communicate the knowledge acquired clearly, using adequate and rigorous terminology. *Capacities to continue learning* Ability to autonomously deepen the notions of physical chemistry and to identify the interconnection between the subjects of study.
Contents	Principles of Thermodynamics, Chemical Kinetics and Spectroscopy
Course program	**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.
Bibliography	P.W. Atkins, J. De Paula. Elements of Physical Chemistry, Zanichelli (Bologna) P.W. Atkins Physical Chemistry Zanichelli (Bologna)
Notes	Publishing House Website
Teaching methods	The course includes lectures with the support of PowerPoint presentations and exercises in the classroom and / or on the TEAMS platform.
Assessment methods	Written and oral exam on all the topics of the program.
Evaluation criteria	• *Knowledge and understanding* Students must demonstrate that 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 to master the basic chemical-physical principles acquired. • *Communication skills* Students must be able to express the acquired knowledge in written and oral form, in a clear and rigorous way. • *Capacities to continue learning* Students must demonstrate that they have acquired the fundamental notions in a critical way and that they are able to identify interconnections and applications of the acquired concepts in real contexts.
Further information	