UNIVERSITÀ DEGLI STUDI DI PALERMO

DEPARTMENT	Scienze e Tecnologie Biologiche, Chimiche e Farmaceutiche
ACADEMIC YEAR	2023/2024
BACHELOR'S DEGREE (BSC)	CHEMISTRY
INTEGRATED COURSE	PHYSICAL CHEMISTRY III WITH LABORATORY
CODE	13737
MODULES	Yes
NUMBER OF MODULES	2
SCIENTIFIC SECTOR(S)	CHIM/02
HEAD PROFESSOR(S)	CHILLURA MARTINO DELIA FRANCESCA — Professore Ordinario — Univ. di PALERMO
OTHER PROFESSOR(S)	FERRANTE FRANCESCO — Professore Associato — Univ. di PALERMO CHILLURA MARTINO DELIA FRANCESCA — Professore Ordinario — Univ. di PALERMO
CREDITS	10
PROPAEDEUTICAL SUBJECTS	00133 - GENERAL AND INORGANIC CHEMISTRY 15248 - CHEMICAL PREPARATIONS WITH LABORATORY PRACTICE
MUTUALIZATION	
YEAR	3
TERM (SEMESTER)	2° semester
ATTENDANCE	Mandatory
EVALUATION	Out of 30
TEACHER OFFICE HOURS	**CHILLURA MARTINO DELIA FRANCESCA** Monday 15:00 16:00 Studio Prof. Chillura. Ed. 17 - Viale delle Scienze **FERRANTE FRANCESCO** Tuesday 14:00 18:00 Viale delle Scienze, edificio 17, ufficio P1080 Thursday 14:00 18:00 Viale delle Scienze, edificio 17, ufficio P1080

DOCENTE: Prof.ssa DELIA FRANCESCA CHILLURA MARTINO

PREREQUISITES	Basic concepts of classical physics. Principles of classical thermodynamics of equilibrium ideal and non-ideal systems.
LEARNING OUTCOMES	1.Content knowledge and understanding Acquisition of basic concepts of quantum mechanics and of spectroscopy for understanding the connection between microscopic and macroscopic properties of matter. Skill in using the specific terms of the subject. Application skills of appropriate theoretical models for the investigation of thermodynamic and structural properties even in connection to computational limitations. Knowledge of the laws ruling intermolecular interactions, the basic principles of Thermodynamics, Quantum Mechanics (MQ) and Spectroscopy. 2. Skill in applying content knowledge and understanding Ability in recognizing the essential features and microscopic interactions useful in interpreting and predicting the macroscopic behaviour. 3. Judgment autonomy Ability in evaluating the implications of a model-based approach. Skill in applying knowledge of quantum mechanics, thermodynamical principles and spectroscopy to specific problems. Skill in carrying out experiments in thermodynamics, kinetics, quantum mechanics and spectroscopy by using in a responsible manner advanced scientific equipment. Ability to formulate independent opinions on scientific problems, to carry out experiments and to interpret experimental data. 4.Communications skills Ability in illustrating, even to a non-specialized audience, the limitations and the advantages of alternative interpretation models. Ability to express the importance of using microscopic models and specific applications. Ability in expressing in a concise and original fashion the relevant concepts. 5. Learning skills A high level of balanced learning skills allowing to tackle specialized studies in an independent way is expected.
ASSESSMENT METHODS	Oral examination including discussion of laboratory reports. Assessment is based on a thirty grade scale. Description of the evaluation methods: Excellent, 30-30 e lode, excellent contents knowledge, excellent use of the language, good analytical skill, the student is capable of applying content knowledge in order to solve proposed problems; very good, 26-29, good contents knowledge, full familiarity with specific language, the student is capable of applying content knowledge in order to solve proposed problems; good, 24-25, basic knowledge of main topics, fair use of the language, with a limited ability of applying content knowledge in order to solve independently proposed problems; fair, 21-23, the student does not show full competence on the main topics of the subject, but he shows content knowledge, fair use of the language, poor ability in applying independently the acquired knowledge; sufficient, 18-20, minimum basic content knowledge of the main topics of the subject and of the technical terms, very poor or nonexistent ability in applying independently the acquired knowledge; fail, the students does not show an acceptable content knowledge of the topics dealt with in the course. The overall evaluation is the weight by CFU of the assessments of the modules.
TEACHING METHODS	Lectures (module 1), laboratory experiments (module 2)

MODULE
PHYSICAL CHEMISTRY III

Prof. FRANCESCO FERRANTE

SUGGESTED BIBLIOGRAPHY

Fondamentali:
- I postulati della Meccanica Quantistica (dispense fornite dal docente)
- Fondamenti di Termodinamica Statistica (dispense fornite dal docente)
- Elementi di Spettroscopia Molecolare (dispense fornite dal docente)

Testi di approfondimento:
D.A. McQuarrie, Statistical Mechanics, Harper & Row
J. M. Hollas, Modern Spectroscopy, Wiley

AMBIT	50135-Discipline chimiche inorganiche e chimico-fisiche
INDIVIDUAL STUDY (Hrs)	102
COURSE ACTIVITY (Hrs)	48

EDUCATIONAL OBJECTIVES OF THE MODULE

The main purpose of the module is to give to the students the fundamental theoretical concepts of quantum mechanics and statistical thermodynamics, as well as to define the role these theories have inside the spectroscopic techniques. The student will learn the axiomatic formulation of quantum mechanics, the quantum description of translation, rotational and vibrational motions, the quantization of energy and the definition of a quantum state. He/she will acquire the statistical definition of the states of a system formed by a huge number of particles, the rules which govern the distribution of particles among the energy levels and the connection between the macroscopic properties of a system and its microscopic composition, through the partition function. He/she will be able to comprehend the rules affecting the position and the intensity of a peak in a spectrum and to foresee the rotational and vibrational spectra of simple molecules. He/she will be able to use the concepts he/she learned in other courses and future studies.

SYLLABUS

Hrs	Frontal teaching
2	Introduction to quantum mechanics. The failure of classical physics: the black body radiation, the heat capacity of solids, the fotoelectric effect, the hydrogen atom spectrum, the electron diffraction.
4	Complements of math: N-dimensional complex vector spaces, linear transformations, eigenvalue equations.
4	The postulates of quantum mechanics. The wavefunction and the Born interpretation, the quantum operators, the expectation value of an observable, the Schroedinger equation, the stationary states.
10	The solution of the Schroedinger equation for systems with centrosymmetrical potential. The free particle, the Heisenberg principle, the quantum tunnel effect and its role in the interpretation of some experimental evidences. The particle in a hole, the quantization of energy, the degeneracy of energy levels. The correspondence principle. The rigid rotor, the quantization of angular moment. The harmonic oscillator. The hydrogenoid atoms and the atomic orbitals.
2	Quantum explanation of experimental findings not interpretable by classical mechanics.
2	Introduction to statistical thermodynamics. Connection between macroscopic properties and microscopic composition of systems.
4	Definition of microstates and macrostates. Boltzmann statistics. The partition function and its properties.
4	Definition of entropy according to Boltzmann, connection with the second and the third principles of thermodynamics. Statistical interpretation of energy flow in the form of work and heat. Statistical expressions for thermodynamic functions.
4	Introduction to spectroscopy. The electromagnetic spectrum and the interaction of matter with radiation. The transition probability; the transition dipole moment and the selection rules. Factors that affects the peaks' width.
4	Rotational spectroscopy, factors affecting the position and the intensity of peaks. Rotational selection rules. Simulation of the rotational spectrum of a diatomic molecule. Informations that can be extracted from a rotational spectrum.
4	Vibrational spectroscopy. Vibrational selection rules. Basics on normal mode of vibration. Simulation of the vibrational spectrum of a polyatomic molecule.
2	Atomic spectroscopy. The transitions which are responsible of the colors at the flame.
2	Molecular electron spectroscopy. Selection rules. Franck-Condon factors. Fluorescence and phosphorescence.

MODULE
PHYSICAL CHEMISTRY III - LABORATORY

Prof.ssa DELIA FRANCESCA CHILLURA MARTINO

SUGGESTED BIBLIOGRAPHY	
I testi adottati nei tre corsi teorici di Chimica Fisica Materiale fornito dal docente	
AMBIT	10693-Attività formative affini o integrative
INDIVIDUAL STUDY (Hrs)	47
COURSE ACTIVITY (Hrs)	53

EDUCATIONAL OBJECTIVES OF THE MODULE

The module aims to apply the concepts acquired within the course of Physical Chemistry III. Each student will perform 3 experiments. The approach is based on problem-solving methodology. The activities will be presented to the class by applying the above methodology. The results of the experiences will be discussed collegially based on the approach of circular didactics.

SYLLABUS

Hrs	Frontal teaching
1	Introduction and purpose of the module. Chronoprogram of the experiences. Organization of the laboratory groups and of their schedule.
1	Methods of preparation of laboratory reports. Security standards to be observed in the laboratory.
5	Illustration of experience and description of scientific equipment.
1	Basic concepts of error propagation.

Hrs	Workshops
10	Structure of matter: determination the size of particles dispersed in a solvent by dynamic light scattering. Alternatively, based on the availability of the instrumentation, this experience will be replaced with the determination of the crystalline structure by X-ray diffraction. Execution of the experience and drafting of the laboratory report.
10	Structure of matter: acquisition and interpretation of ATR-FT-IR spectra. Execution of the experience and drafting of the laboratory report.
10	Quantum Mechanics: Calculation of the vibrational structure of the first band of the electronic spectrum, absorption and fluorescence of a diatomic molecule. Execution of the experience and drafting of the laboratory report.
15	Discussion of results: literature comparison, critical evaluation of the validity of the results and of their application to a research oriented contest. Preparation and presentation of a short powerpoint concerning the laboratory activities.