Physical Chemistry-2

1. GENERAL

SCHOOL	NATURAL SCIENCES		
ACADEMIC UNIT	CHEMISTRY		
LEVEL OF STUDIES	UNDERGRADUATE		
COURSE CODE	**XA339**	**SEMESTER**	**3rd**
COURSE TITLE	PHYSICAL CHEMISTRY-2		

INDEPENDENT TEACHING ACTIVITIES *if credits are awarded for separate components of the course, e.g. lectures, laboratory exercises, etc. If the credits are awarded for the whole of the course, give the weekly teaching hours and the total credits*	**WEEKLY TEACHING HOURS**	**CREDITS**
Lectures	3	5
Seminars	1	
Laboratory work	-	
Add rows if necessary. The organisation of teaching and the teaching methods used are described in detail at (d).		

COURSE TYPE *general background, special background, specialised general knowledge, skills development*	Field of Science (Physical Chemistry).
PREREQUISITE COURSES:	There are no prerequisite courses.
LANGUAGE OF INSTRUCTION and EXAMINATIONS:	Greek. However, the course can be taught in English if foreign students are enrolled.
IS THE COURSE OFFERED TO ERASMUS STUDENTS	YES
COURSE WEBSITE (URL)	

2. LEARNING OUTCOMES

Learning outcomes

The course learning outcomes, specific knowledge, skills and competences of an appropriate level, which the students will acquire with the successful completion of the course are described.

Consult Appendix A

- *Description of the level of learning outcomes for each qualifications cycle, according to the Qualifications Framework of the European Higher Education Area*
- *Descriptors for Levels 6, 7 & 8 of the European Qualifications Framework for Lifelong Learning and Appendix B*
- *Guidelines for writing Learning Outcomes*

At the end of the course the student will be able to have basic knowledge for the interpretation of spectroscopic observations and measurements.

General Competences

Taking into consideration the general competences that the degree-holder must acquire (as these appear in the Diploma Supplement and appear below), at which of the following does the course aim?

Search for, analysis and synthesis of data and information, with the use of the necessary technology	*Project planning and management*
Adapting to new situations	*Respect for difference and multiculturalism*
Decision-making	*Respect for the natural environment*
Working independently	*Showing social, professional and ethical responsibility and sensitivity to gender issues*
Team work	*Criticism and self-criticism*
Working in an international environment	*Production of free, creative and inductive thinking*

Working in an interdisciplinary environment *Production of new research ideas*	*Others*

At the end of this course the student will further develop the following skills:

Using advanced specialized software in applications in Chemistry: Spectroscopy, Molecular Modelling in Organic and Inorganic Chemistry.

3. SYLLABUS

- Historical introduction. The discovery of th electron by J.J. Thomson. Black body radiation and classical physics. Planck's Law. The electronic spectrum of the hydrogen atom. Rydberg's equation. Quantization of the angular momentum and Bohr's model of the hydrogen atom. De Broglie's theory, wave properties of matter. Heisenberg's Uncertainty Principle.
- The wave equation. The vibrating spring. Solving the wave equation by variable separation. General solution of the wave equation.
- Schrödinger's equation and some simple problems. Solving Schrödinger's equation: an eigenvalue problem. Observables and linear operators in Quantum Mechanics. A particle in a potential well: energy quantization. Uncertainty principle for a particle in a potential well.
- General principles of quantum Mechanics. The state of a system. Linear operators in Quantum Mechanics. Time-dependence of the wavefunction. Quantum mechanical operators, commutation and the uncertainty principle.
- The harmonic oscillator. Schrödinger's equation and energy levels. Infrared spectra of diatomic molecules. Asymptotic solution of Schrödinger's equation.
- Three-dimensional problems. Particle-in-a-box. Separable hamilto-nian operators and the corresponding wavefuctions. Schrödinger's equation for the hydrogen atom. Symmetry of s orbitals. Schrödinger's equation for the helim atom.
- Approximative methods. Perturbation theory. The variational principle.
- Atoms. Atomic units system. Studying the helium atom. Hartree-Fock equations and the self-consistent field method. Antisymmetric wavefunctions. Hartree-Fock calculations and comparison with experimental data.

4. TEACHING and LEARNING METHODS - EVALUATION

DELIVERY *Face-to-face, Distance learning, etc.*	Lectures and seminars face-to-face.
USE OF INFORMATION AND COMMUNICATIONS TECHNOLOGY *Use of ICT in teaching, laboratory education, communication with students*	Use of Information and Communication Technologies (ICTs) (PowerPoint) in Lectures. Seminars. Problems are solved in an exemplary way. The course includes practical exercises through the application of specialized software for the study of basic characteristics of atoms and molecules.
TEACHING METHODS *The manner and methods of teaching are described in detail.* *Lectures, seminars, laboratory practice, fieldwork, study and analysis of bibliography, tutorials, placements, clinical practice, art workshop, interactive teaching, educational visits, project, essay writing, artistic creativity, etc.* *The student's study hours for each learning activity are given as well as the hours of non-directed study according to the principles of the ECTS*	(see table below)

Activity	*Semester workload*
Lectures (3 contact hours per week x 13 weeks)	39
Seminars (1 contact hour per week x 13 weeks) - solving of representative problems	13
Final written examination (3 contact hours)	3
Private study time of the student and preparation for final examination	70
Course total	***125***

STUDENT PERFORMANCE EVALUATION *Description of the evaluation procedure*	One written examination at end of Semester 100% of grade. Minimum passing grade: 5.

Language of evaluation, methods of evaluation, summative or conclusive, multiple choice questionnaires, short-answer questions, open-ended questions, problem solving, written work, essay/report, oral examination, public presentation, laboratory work, clinical examination of patient, art interpretation, other *Specifically-defined evaluation criteria are given, and if and where they are accessible to students.*	

5. ATTACHED BIBLIOGRAPHY

1. D. A. McQuarrie, "*Quantum Chemistry*", University Science Books, 1983.
2. C. J. Cramer, "*Computational Chemistry: theories and models*", Wiley, 2004.