YOZGAT BOZOK UNIVERSITY FACULTY OF ARTS AND SCIENCES

CHEMISTRY DEPARTMENT COURSE PLAN

Course Code	Course Title	Semester	Course Type (C/E)	T+A+L (Time/Week)	Credit	ECTS	Course Language
KİM474	QUANTUM CHEMISTRY	FALL	C	2+0+0		4	Turkish

COURSE INFORMATION

Course Catalog Description (Content)	Events supporting quantum chemistry; black body radiation; photoelectric effect; atomic spectra; Schrodinger equation; characteristics of operators; postulates of quantum mechanics; applying the principles of quantum mechanics to simple systems; two-particle systems; electronic structure of atoms; introduction to molecular structure
The Aim of the Course	To give students the ability to explain and interpret chemical phenomena.
Course Level	Bachelor degree
Course Language	Turkish
Teaching method	(X) Formal ( ) Online ( ) Mixed/Hybrid
Teaching Staff of the Course	Prof. Dr. Dr. Ramazan COŞKUN, Prof. Dr. Ali DELIBAŞ, Asst. Prof. Dr. Hatice ARI
Prerequisite Course(s) of the Course	-
Learning Outcomes from the Course	**1-** Make use of the principles of quantum mechanics, and apply these principles to atoms and molecules. **2-** Interpret atomic and molecular spectra. **3-** Calculate the properties of substances. **4-** Will be able to determine the reactivity of substances under different conditions. **5-** Can explain all chemical events.

COURSE CONTENT

Week	Theory	Practice/Laboratory
1	Introduction to quantum chemistry: structure of matter; electromagnetic radiation; black body radiation; photoelectric effect	
2	Atomic spectra; spectrum of the hydrogen atom; Bohr atomic model; De Broglie relation; classical wave equation; Schrodinger equation; wave function	
3	Principles of quantum mechanics: postulates of quantum mechanics; operators; eigenvalue and Schrodinger equation; eigenvalue spectrum and degeneration	
4	Application of quantum mechanics principles to simple systems: rules; free particle; a particle in a one-dimensional box; Heisenberg uncertainty principle; particle in a three-dimensional box; two-body problems; rigid rotor.	
5	Structure of the atom: hydrogen atom; quantum numbers	
6	Orbital shapes; spin quantum numbers; multi-electron atoms	

7	Molecular structure: Born-Oppenheimer approach; Schrodinger equations of molecules; linear combination of atomic orbitals; Hückel approaches; Molecular orbitals of H2+	
8	Covalent bond and its types; approach; Application areas of molecular orbital calculations	
9	Orbital symmetry and its application to reactions: symmetry elements and symmetry operations; orbital symmetry; Woodward-Hoffmann approach	
10	Electrocyclic reactions	
11	Cycloaddition reactions	
12	Principles of spectroscopy: Nuclear movements; harmonic oscillator; tunnel effect	
13	Molecular vibration and rotational movements	
14	Rotation spectra; vibration-rotational spectra; electronic spectra	
15	Final Exam	

Course Learning Resources

1. Karaoğlu, B., Kuantum Mekaniğine Giriş, Bilgi Tek Publishing, Istanbul, 1994.
2. Çınar, Z., Kuantum Kimyası, Bookstore, Istanbul, 1994.
3. Levine, I.N., Quantum Chemistry, Prentice-Hall, Englewood Cliffs, 1991.
4. McQuarrie, D.A., Quantum Chemistry, University Science Boks, Mill Valley, 1983.
5. Atkins, P.W., Molecular Quantum Mechanics, Oxford University Press, New York, 1983.

ASSESSMENT CRITERIA

Work Activities During the Semester	Number	Contribution
Homework	1	30
Practice		
Forum/ Discussion Application		
Short Exam (Quiz)	2	70
Ratio Of Semester Studies To Semester Success (%)		%40
Ratio of Final to Success (%)	**1**	%60
Total		%100

COURSE WORKLOAD TABLE

Activity	Total Weeks	Duration (Weekly Hours)	Total Workload
Theory	14	2	28
Practice			
Forum/ Discussion Application			
Reading	14	2	28
Internet Scanning, Library Study	14	2	28
Material Design, Application			
Report Preparation			
Presentation Preparation			
Presentation			
Final Exam	1	1	1
Preparation for the Final Exam	3	5	15
Other(s) (Specify: … …. ……..)			

Total Workload	100
Total Workload / 25 (s)	100/25
ECTS Credits of the Course	≅4
Note: The workload of the course will be determined by the instructor on a per-course basis.	

PROGRAM LEARNING OUTPUTS CONTRIBUTION LEVELS

No	Program Learning Outputs	1	2	3	4	5
1	Gains extensive knowledge about the basic chemical properties of matter and uses this knowledge in daily life, industrial scale, and practical chemistry and shares them with the society.			**x**		
2	Performs experiments, collects data, interprets, evaluates results, defines problems parallel to current technological developments, produces solutions against problems encountered in the laboratory.			**x**		
3	Calculates and processes chemical information and data.					**x**
4	Applies her/his knowledge and understanding of chemistry to the solution of unconventional qualitative and quantitative problems.				**x**	
5	Defines and comprehends chemical concepts and theories in Inorganic Chemistry, Organic Chemistry, Physical Chemistry, Analytical Chemistry, Biochemistry.				**x**	
6	Can conduct research in the light of scientific data on any subject in the field of chemistry.				**x**	
7	Writes, presents, discusses scientific material, and presents it orally to a knowledgeable audience.			**x**		
8	Brings a chemical approach to the solution of environmental problems, makes environmental analyzes and reports.		**x**			
9	Knows a foreign language at a level to read and understand the basic terms and processes of the chemist profession.		**x**			
10	Can use computer software and information and communication technologies at the level required by the field.					**x**
11	Adapts and transfers the knowledge gained in the field to secondary education.		**x**			
12	Apart from the field of chemistry, she/he gains knowledge in different branches of science that she feels close to.					**x**
13	Carries out a study independently, makes group work and gains the awareness of taking responsibility.			**x**		
14	They can develop a positive attitude towards lifelong learning and constantly renew their professional knowledge and skills.				**x**	
15	Have sufficient awareness of the universality of social rights, social justice, quality culture and protection of cultural values, environmental protection, occupational health and safety.	**x**				