Kingdom of Saudi Arabia

National Commission for Academic Accreditation & Assessment

COURSE SPECIFICATION

Quantum Chemistry

Chem 436

Revised

Thursday, 23 October 2014

Course Specification

Institution:	**King Khalid University**
College:	**College of Science**
Department:	**Department of Chemistry**

A. Course Identification and General Information

1. Course title and code: **Quantum Chemistry (Chem 436)**
2. Credit hours: **2**
3. Program(s) in which the course is offered: **Bachelor of Science of Chemistry**
4. Name of faculty member responsible for the course: **Dr. Morad Mustafa**
5. Year or Level at which this course is offered: **Year 4 (Level 8)**
6. Pre-requisites for this course (if any): **General Chemistry (Chem 101) and Mathematics (Math 101)**
7. Co-requisites for this course (if any): **None**

8. Location (if not on main campus):

Main Campus

B. Objectives

1. Summary of the main learning outcomes for students enrolled in the course.

- **Understand the concepts of basic principles of quantum chemistry.**
- **Understand the failures of classical physics.**
- **Learn how to deal with the concept of operators and eigenvalue problems.**
- **Understand the postulates of quantum mechanics.**
- **Learn how to compute probabilities, expectation values, and commutators.**
- **Learn how to solve the appropriate Schrödinger equations for a variety of systems.**
- **Apply the Schrödinger equation to a variety of standard cases (Translational, Vibrational, and Rotational motions).**
- **Describe the electronic structure of hydrogen-like atoms.**
- **Describe the electronic structure of many-electron atoms.**

2. Briefly describe any plans for developing and improving the course that are being implemented.

- **Diversify teaching methods, such as using models and showing animation for explaining difficult concepts.**
- **Continuous development to keep the contents of this course updated with the results of modern scientific research.**
- **Activation of more e-learning with this course by the University's website.**

C. Course Description

1.1. Topics to be covered in the theoretical course.

Topics	No. of Weeks	Contact Hours
Course Introduction	**0.5**	**1**
Mathematical Background Review **Coordinate Systems** **Logarithms and Exponentials** **Differentiation and Integration** **Partial Derivatives** **Differential Equations** **Complex Numbers** **Matrices** **Vectors**		
The Origins of Quantum Mechanics **Introduction** **Black-body Radiation** **Heat Capacities** **Quantization** **The Photoelectric Effect** **Atomic Spectra** **The Duality of Matter**	**1**	**2**
The Principles of Quantum Mechanics **Introduction** **Operators in Quantum Mechanics** **The Postulates of Quantum Mechanics** **The Specification and Evolution of States**	**3**	**6**
Exam 1	**1**	**1**
Linear Motion and the Harmonic Oscillator **Introduction** **The Characteristics of Acceptable Wavefunctions** **Particle in a Box** **Penetration into and through Barriers**	**3**	**6**

Topics	No. of Weeks	Contact Hours
The Harmonic Oscillator		
Exam 2	**1**	**1**
Rotational Motion and the Hydrogen Atom Introduction Particle on a Ring Particle on a Sphere Motion in a Coulombic Field The Structures of Many-Electron Atoms	**3**	**6**
Final Exam		

2. Course components (total contact hours per semester).

Lecture	Tutorial	Laboratory	Practical/Field work/Internship	Other
20	4	0	0	0

3. Additional private study or learning hours (expected for students per week).

- 2 hours for private study.
- 3 hour for homework assignment.

4. Development of Learning Outcomes in Domains of Learning.

a. Knowledge

(i) Description of the knowledge to be acquired

- The concepts of basic principles of quantum chemistry, wave-particle duality, Schrödinger equation and the information in a wavefunction, uncertainty principle, and electronic structures.
- The failures of classical physics.
- The postulates of quantum mechanics.
- The idea behind the models for the Translational, Vibrational, and Rotational motions.
- Electronic structure of hydrogenic atoms.

(ii) Teaching strategies to be used to develop that knowledge

- Lectures.
- Tutorials.
- Dialogue and discussion.

(iii) Methods of assessment of knowledge acquired

- **Two midterm and final exams that consist of the following types of knowledge questions (20% of final assessment): multiple choices, as well as true and false.**
- **Quizzes.**

b. Cognitive Skills

(i) Description of cognitive skills to be developed

- **Solving the appropriate Schrödinger equations to find the properties of systems according to quantum chemistry.**
- **Apply the Schrödinger equation to a variety of standard cases (Translational, Vibrational, and Rotational motions).**
- **Analyze the electronic structure of hydrogenic atoms.**

(ii) Teaching strategies to be used to develop these cognitive skills

- **Explanations and examples given in lectures and practising them under supervision in tutorials.**
- **Dialogue and discussion.**
- **Posting many examples and questions on the web page of the academic course.**
- **Introduce students to the available references in the library and websites specialized in this field.**
- **Demonstrating quantum chemistry principles and applications using software packages.**

(iii) Methods of assessment of students cognitive skills

- **Two midterm and final exams that consist of the following types of cognitive skills questions (60% of final assessment): multiple choices, true and false, and calculate.**
- **Homework assignments.**
- **Quizzes.**

c. Interpersonal Skills and Responsibility

(i) Description of the interpersonal skills and capacity to carry responsibility to be developed

- **Educating student about ethics of dealing with his colleagues and with the instructors and supervisor.**
- **Teaching students the responsibility toward themselves and toward others.**
- **Working in group to make the students aware of responsibility.**
- **Instilling the self-learning character in the student.**
- **Decision-making.**
- **Independence.**
- **Work effectively.**

(ii) Teaching strategies to be used to develop these skills and abilities

- **Distribution students to different groups in the practical lessons to acquire skills of dealing with everyone.**
- **Dialogue and discussion.**

(iii) Methods of assessment of students interpersonal skills and capacity to carry responsibility

- **Assessment of assignments includes portion of grade for effectiveness of investigation processes.**
- **Personal performance in classroom.**

d. Communication, Information Technology and Numerical Skills

(i) Description of the skills to be developed in this domain.

- **The ability to communicate in English both orally and in writing.**
- **Enhancing the knowledge in information technology that will enable them to gather, interpret, and communicate information and ideas.**
- **Providing sufficient information about mathematical techniques that will enable them to apply in interpreting and proposing solutions.**
- **Communicate via the available electronic tools.**
- **The use of search engines across the Web.**

(ii) Teaching strategies to be used to develop these skills

- **Student assignments that require good standards of use of IT and mathematics techniques.**
- **Teaching by using the e-learning tools.**

(iii) Methods of assessment of students numerical and communication skills

- **Two midterm and final exams that consist of the following types of communication skills questions (20% of final assessment): multiple choices, true and false, calculate, and solve.**
- **Homework assignments.**

e. Psychomotor Skills (if applicable)

(i) Description of the psychomotor skills to be developed and the level of performance required

- **Computer typing.**
- **Reading and writing.**

(ii) Teaching strategies to be used to develop these skills
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(iii) Methods of assessment of students psychomotor skills
• **Homework assignments.**

5. Schedule of Assessment Tasks for Students During the Semester.

Assessment	Assessment task	Week due	Proportion of Final Assessment
1	Quizzes	Weekly	10
2	Homework Assignments	Weekly	10
3	First Exam	5	15
4	Second Exam	9	15
6	Final Exam (Open book or closed book)	16	50

D. Student Support

1. Arrangements for availability of teaching staff for individual student consultations and academic advice.
• **Office Hours: 7 hours** • **Help Session: 1 hour**

E. Learning Resources

1. Required Text(s)
• *Molecular Quantum Mechanics* by Peter W. Atkins and Ronald S. Friedman, 2010, 5th ed.

2. Essential References
• *Quantum Chemistry* by Ira N. Levine, 2008, 6th ed. • *Physical Chemistry* by Peter Atkins and Julio dePaula, 2009, 9th ed. • *Quantum Chemistry and Spectroscopy with Mastering Chemistry* by Thomas Engel, 2012, 3rd ed.

3. Recommended Books and Reference Material
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4. Electronic Materials
• E-Learning Deanship (http://elc.kku.edu.sa/en/).

5. Other learning material
• None.

F. Facilities Required

1. Accommodation
• A classroom containing at least 45 seats and equipped with projector and Internet access (scheduled for 2 hours once a week). • A help session classroom containing at least 45 seats and equipped with projector and Internet access (scheduled for 1 hours every week).

2. Computing resources

- **Common computer lab containing at least 25 computer sets.**
- **High speed internet access.**

3. Other resources
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G. Course Evaluation and Improvement Processes

1. Strategies for Obtaining Student Feedback on Effectiveness of Teaching

- **Confidential completion of standard course evaluation questionnaire.**
- **Focused group discussion with small groups of students.**
- **Review with the department chairman.**

2. Other Strategies for Evaluation of Teaching by the Instructor or by the Department

- **Observations and assistance from colleagues.**
- **Independent assessment of standards achieved by students.**
- **Independent advice on assignment tasks.**

3. Processes for Improvement of Teaching

- **Workshops on teaching methods.**
- **Review of recommended teaching strategies.**
- **Periodical department revisions on its methods of teaching by experts on the teaching.**

4. Processes for Verifying Standards of Student Achievement

- **Check marking by an independent member teaching staff of a sample of student work.**
- **Periodic exchange and remarking of tests or a sample of assignments with staff at another institution.**

5. Describe the planning arrangements for periodically reviewing course effectiveness and planning for improvement.

- **Periodic revision of the course from concerned parties in the department and college, and improving it according to what is known in distinguished universities worldwide.**
- **Perform the necessary changes based on the feedback from the statistical analysis of the student grades.**
- **Perform the necessary changes based on the feedback from the workshops, conferences, and seminars recommendations.**
- **Perform the necessary changes based on the feedback from the experts in the field and faculty members.**