Ministry of Higher Education and Scientific research

Department of Chemistry
College of Science
University of Salahaddin

Subject: Quantum Chemistry
Course Book – (4th year)
Lecturer's name: Dr. Shireen Ibrahim Hamadamin
Academic Year: 2019/2020

Course Book

Course name .1	Quantum Chemistry
Lecturer in charge .2	Shireen Ibrahim Hamadamin
3. Department/ College	Chemistry/ Science
4. Contact	Shireenhawlery@gmail.com Drshireenchemistry@gmail.com Shireen.hamadamin@su.edu.krd
5. Time (in hours) per week	The course is Theoretical study without experimental technique. 4th stage: 2 group, total 6hr.
6. Office hours	All the days I am in the Chemistry department
7. Course code	None
Teacher's academic .8 profile	https://sites.google.com/a/su.edu.krd/shireen.hamadamin-2019/

9. Keywords	**None**

10. Course overview:

I believe that quantum mechanics can most logically be introduced to fourth stage of undergraduate students, who usually know very little about the physics of wave motion, by the postulational approach. This approach begins with the classical Hamiltonian and then transforms to the appropriate quantum mechanical operators as is done in the Schrodinger formalism, to understand molecular physics, quantum mechanics and spectroscopy are part of the subject matter of physical chemistry are essential to the chemist's training, so the study will be sufficient and comprehensive. At the end of the .year, the student will gain full knowledge for future employment

11. Course objective:

By the end of the course allow the student to:

- Develop quantum ideas in an undergraduate course in conjunction with some selection of topics from classical physical chemistry.
- Introduction to the mathematical fundamentals, with specific problems.
- Introduce modern quantum mechanical treatments of atoms and molecules more adequately.
- Introduce all the topics of spectroscopy, atomic structure, molecular structure and spectra, the electron and nuclear magnetic resonance spectroscopy, these subjects are developed in a logical sequence.

12. Student's obligation

Students obliged to attend all theoretical lectures for around 32 weeks; quizzes will be given after each chapter completed, three exams are compulsory to sit on November, February and May.

13. Forms of teaching

- Lectures: that covers and explains the chemical concepts mentioned above. All lectures will be presented by the aid of Data show and will be supported by doing the following techniques.
- Solved examples: from the text or from problems set will be given to student.
- Home works, the student must submit a complete report for solutions of the given problems:
- Every sitting exam assigned for the students, question papers displayed on public board, questions are corrected, marks rewarded, and the following lecture will be discussion to solve the exam questionnaire and place a copy of answers on to their notes after giving several ways of answering.
- The corrected papers evaluated and marks displayed. Exam answer papers are to be saved for future references.
- The exam paper covers most of the lectures given and indicated: Exam instructions, MCQ, definitions, chemical equations, explanations, Draw, give reasons, calculations, comparisons…etc. The questions are usually clear, direct and obvious, starting from easy, medium to hard.
- Every class activity for students is to be recorded on lecture notebook, saved as references.
- All student marks including attendance and quizzes shall be displayed on the department notes board. All year student effort will be calculated and added to the summer exam along with the practical marks out of a 100%.
- Students who passed the first attempt summer exam will be granted next level of study.

14. Assessment scheme

The whole year marks out of 100%, (breaking down to 40 marks for exams including .quizzes and classroom activity) plus 60 mark for final Summer examination

:Student learning outcome .15

The students will learn from the lecturer, and other sources of information including the educational websites, books from the library, etc.

16. Course Reading List and References:

Required book:

1- Fundamentals of quantum chemistry. By James E. House, 2nd Edition, Elsevier science (USA), 2004.

2- Physical chemistry, F. Daniels R. A. Alberty, 3rd Edition, John Wiley & Sons, inc. 1966.

3- Physical chemistry, Atkins & de paula, 7th ed., Oxford University press, 2007.

4- Quantum mechanics in chemistry, Melvin W. Hanna, 2nd ed., W. A. Benjamin, Inc., 1969.

5- Basic quantum chemistry, Leon F. Phillips, 3rd Edition, John Wiley & Sons, inc. 1965.

6- Quantum chemistry methods and applications, R. Daudel, R. Lefebvre and C. Moser, 2nd Edition, John Wiley & Sons, inc. 1965.

7- Molecular quantum mechanics, P.W. Atkins, 2nd edition, clarendon press, oxford, 1970.

:The Topics .17	**Lecturer's name**
Course Outline	Dr. Shireen Ibrahim Hamadamin

Chapter 1

(2)weeks
(1)Lec.
Discussion

1.1 Physical chemistry
1.2 Coordinate system
1.3 Matrices
1.4 Determinates
1.5 Complex Number (c)
1.6 Operator
1.7 Eigen value equation
1.8 Integration

Chapter 2

(3)weeks
(1)Lec.
Discussion

2.1 Classical mechanics
2.2 LaGrange equation and LaGrange function
2.3 Hamiltonian function and Hamiltonian equation of motion
2.4 Internal coordinates and the motion of the centre of mass.
2.5 The basic assumptions of the classical mechanics

Chapter 3

(3)weeks
(1)Lec.
Discussion

3.1 Old Quantum theory
3.1.1 Black body radiation
3.1.2 Photoelectric effect
3.1.3 The Compton effect
3.1.4 Atomic models and spectra
3.2 Matter waves

Chapter 4

(7)weeks
(1)Lec.
Discussion

4.1 Quantum mechanical
4.1.1 Dynamic variable
4.1.2 Postulates
4.2 Normalization of wave functions
4.3 Orthogonality
4.4 Application of the postulated to simple systems
4.5 Correspondence principle
4.6 Comparison between classical mechanics and quantum mechanics for a particle in a box
4.7 A particle in three dimensional
4.8 Particle in a ring
4.9 The condition for normalization
4.10 The hydrogen atom and (Hydrogen like atom)

	Second course **Chapter one** 1.1 Spectroscopy 1.2 Region spectrum 1.3 Spectrophotometer
(2)weeks (1)Lec. Discussion	1.4 Beer-Lambert law **Chapter two** 2.1 Nuclear magnetic resonance 2.2 NMR spectrophotometer 2.3 chemical shift 2.4 Spin-Spin coupling
(2)weeks (1)Lec. Discussion	**Chapter three** 3.1 Electron spin resonance spectroscopy 3.2 Difference between ESR and NMR
(2)weeks (1)Lec. Discussion	**Chapter four** 4.1 Rotational spectroscopy (microwave spectroscopy) 4.2 Rotation of rigid diatomic molecule 4.3 Microwave apparatus, and applications
(2)weeks (1)Lec. Discussion	**Chapter five** 5.1 IR (vibrational) spectroscopy 5.2 vibration- Rotation spectroscopy
	Chapter six 6.1 Raman spectroscopy
(2)weeks (1)Lec. Discussion	**Chapter seven** 7.1 Electronic spectroscopy
	Chapter eight
(2)weeks	8.1 mass spectroscopy
	Chapter nine
(1)week	9.1 Moss-Bauer Spectroscopy (gamma-ray spectroscopy)
(1)week	
(1)week	

18. Practical Topics (If there is any)	
None	

19. Examinations: Theory

(Answer all questions for each question 10 marks)

Q1/a) How much energy is released when an electron falls from the n=4 to the n=2 energy level inside a hydrogen atom? **b)** what is the frequency of this photon? **c)** calculate the wavelength in nm. (planks constant = J.s Speed of light = m/s)

Q2/ fill the following blanks:

1. For the equation , If is the operator for the function (x) then (a) is----------.
2. Identity matrix: if the diagonal element equal to ----------.
3. Classical mechanics could not explain some microscopic phenomena like ----------, ----------, ----------and ----------.
4. The Lagrange equation then Hamilton equation is ----------.
5. In postulate (II): for every observable property of a system there exists a corresponding ----------, ---------- operator.
6. If the two operators are ----------.

Q3/A/Show that the function an eigen function of operator and what is the eigen value?

B/Compute the wave length of an electron (m = moving at (.

Q4/ Draw the coordinates for the hydrogen atom problem and set up the Schrodinger equation with identification of every symbols for hydrogen atom system.

20. Extra notes:
None.

21. Peer review پێداچوونەوەی هاوەڵ
This course book has to be reviewed and signed by a peer. The peer approves the contents of your course book by writing few sentences in this section.
(A peer is person who has enough knowledge about the subject you are teaching, he/she has to be a professor, assistant professor, a lecturer or an expert in the field of your subject).
ئەم کۆرسبووکە دەبێت لەلایەن هاوەڵێکی ئەکادیمیەوە سەیر بکرێت و ناوەڕۆکی بابەتەکانی کۆرسەکە پەسەند بکات و جەند ووشەیەک بنووسێت لەسەر شیاوی ناوەڕۆکی کۆرسەکە و واژووی لەسەر بکات.
هاوەڵ ئەو کەسەیە کە زانیاری هەبێت لەسەر کۆرسەکە و دەبیت پلەی زانستی لە ماموّستا کەمتر نەبێت.