Birla Institute of Technology & Science, Pilani
Hyderabad Campus

FIRST SEMESTER 2022-2023
Course Handout Part II

Date: 29/08/2022

In addition to Part I (General Handout for all courses appended to the timetable), this portion gives further details regarding the course:

Course No. : **CHEM F213**
Course Title : **Physical Chemistry-II**
Instructor-in charge : **Mudit Dixit**
Instructors : **Prof. K. Sumithra and Dr. Mudit Dixit**

Scope and Objectives: The main objectives of this course are to (i) introduce basic principles of quantum mechanics (ii) apply the principles of quantum mechanics to standard problems in the electronic structure of atoms (iii) demonstrate the applicability of Quantum Mechanics on molecules and chemical bonding (Valance Bond and Molecular Orbits theories) (iv) explain the utility of quantum mechanics for explaining the electronic (spin, term symbols) and magnetic (angular momentum) properties of atoms and molecules (v) discuss some approximate methods (Variation and Perturbation methods) for molecules (iv) Illustrate principles of Molecular spectroscopy.

Course Description: This course will begin with the discussion and introduction of the historical development of Quantum Theory and its fundamental principles. Later, these principles will be applied to a series of exactly solvable problems of Quantum Mechanics. In subsequent lectures, Approximate Methods and their application to many-electron atoms will be discussed. The further lectures will discuss theories of chemical bonding (MO, VB, and Huckel) on molecules and spectroscopic methods.

Text Books:

TB1: 'Quantum Chemistry', Donald A. McQuarrie, University Science Books (First Indian Edition 2003, Viva Books Private Limited).

TB2: "Quantum Chemistry", Donald A. McQuarrie, University Science Books, 2nd International Ed., 2008

Reference Books:

(a) 'Quantum Chemistry', Ira N Levine, 5th ed., PHI (2008).
(b) 'Physical Chemistry', P W Atkins & Julio de Paula, 8th ed., OUP (2006).
(c) 'Introduction to Quantum Mechanics with applications to Chemistry', Linus Pauling and E. Bright Wilson, Jr., Dover (1962).
(d) 'Molecular Quantum Mechanics', P W Atkins & Ronald Friedman, 5th ed., OUP (2011)

Course Plan:

Lect. No.	*Topics to be covered*	*Learning Objectives*	*Chapter in the Text Book*
	Development of Quantum Theory		
1-2	Origins of Quantum Theory	Blackbody Radiation, Photoelectric Effect, Atomic Vibration in Crystals, Line Spectra & Bohr Model of H Atom.	**TB1** or **TB2** 1.1-

			1.10
3	Wave-Particle Duality	De Broglie’s postulate, Heisenberg Uncertainty Principle	**TB1** or **TB2** 1.11-1.14
4-5	The Wave Equation	Normal modes, superposition, Fourier series	**TB1** or **TB2** 2.1-2.5
6-8	Postulates of Quantum Mechanics	The wave function, Operators and Observables, Schrodinger equation, Time Evolution, and the Stationary States, Uncertainty	**TB1** 3.1-3.4, 3.7,8,11, 4.1-4.9 or **TB2** 3.1-3.4, 3.7-3.9
	Some Exactly Solvable Problems		
9-10	Particle in a Box	Bound States, Zero Point Energy, Symmetry, Superposition States, Degeneracy in 2 and 3 dimensions	**TB1** 3.4-3.11, 6.1-6.2 or **TB2** 3.4-3.9
11-12	Finite Potential Wells and Barriers	The bound States in Wells, Probability Current, Reflection, and Tunneling	Class Notes, Ref (b) 12.3
13-15	Harmonic Oscillator	Eigenstates, Molecular Vibration	**TB1** 5.1-5.13 or **TB2** 5.1-5.12
16-18	Angular Momentum and Rigid Rotator	Energy levels, Commutation Relations, and Wavefunctions, Molecular Rotation	**TB1** 6.3-6.7, 6.10 or **TB2** MathChapeter E, 6.8, Appendix 6
19-20	The Hydrogen atom	Energy levels, Wavefunctions – Angular and Radial Parts, Orbitals	**TB1** 6.8-6.11 or **TB2** 7.1-7.8
	Approximation Methods		
21-23	Variation Method	Variation theorem, application including Linear Variation	**TB1** 6.12, 7.3-7.7, 8.1,2 or **TB2** 7.9**,** 8.1-8.3
24-25	Stationary State Perturbation Theory	Systematic Correction of Wavefunctions and Energies, Treatment of Degenerate States	**TB1** 7.1,2, 8.2 or **TB2**

			8.4-8.5, Ref (a) 9.1-7
	Many Electron Atoms		
26-27	Many Electron Wavefunctions	Systems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants	**TB1** 8.4-6 or **TB2** 9.4-9.5
28	Atomic Terms and Spectra	Addition of Angular Momenta (S.S), Spin-Orbit Interaction (S.S), Selection Rules	**TB1** 8.9-8.12 or **TB2** 9.9-9.13
	Molecules		
29	Born-Oppenheimer Approximation	Separation of nuclear and electronic motion	**TB1** 9.1 or **TB2** 10.1
30-31	Valence Bond Theory – H_2	Localized Electron Pair Bonds	**TB1** 9.2-9.5 or **TB2** 10.2-10.3
32-33	Molecular Orbital Theory – H_2^+, H_2	Linear Combination of Atomic Orbitals, Comparison to VB Picture	**TB1** 9.6-9.8 or **TB2** 10.4-10.8
34-35	Homonuclear Diatomic Molecules	Molecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms	**TB1** 9.9-9.15 or **TB2** 11.1-11.2
36-37	Hückel MO theory	π-electron approximation for conjugated systems, energies and delocalization, charge distribution, and bond orders	**TB1** 9.21-9.24 or **TB2** 11.6 -11.8
38-40	Molecular Spectroscopy	Vibration-Rotation Spectra, Selection Rules, Electronic Spectra, and the Franck-Condon Principle	**TB1** 10.1-10.18

Expected Learning outcomes:

Lectures	*Learning outcome*
1-2	Discuss historical developments and the need for quantum theory, Spell the mathematical background for quantum theory
3-5	Define and consolidate new concepts to be used in quantum mechanics
6-8	Define the quantum mechanical postulates to make use of in the application
9-10	Apply quantization of states and zero-point energy in very simple systems, like, PIAB
11-12	Solve bound states in potential wells and Identify the working principle of STM
13-15	Define and interpret vibrational spectroscopy of molecules.
16-18	Define and solve rigid rotator as a model for rotating diatomic molecules
19-20	Identify atomic orbital picture of H-atom from quantum mechanics.
21-23	Evaluate the upper bound to the ground state energy of a system employing model systems.
24-25	Estimate ground state energy of various systems from the unperturbed state of the system
26	Identify spin as another coordinate.

27-28	Examine the allowed and forbidden transition in atoms
29	Express molecular wavefunction as a product of nuclear and electronic wavefunctions
30-31	Demonstrate successful description of chemical bond
32-33	Examine the application of molecular orbital theory to diatomic molecules
34-35	Compare experimental observations along with theoretical prediction for diatomic molecules
36-37	Explore the quantum chemical approximation of aromatic systems.
38	Discuss quantum-mechanical approach for spectroscopy. Explain rotational and vibrational spectroscopy
39	Recognize the fundamentals of electronic spectroscopy.
40	Formulate the allowed and forbidden transition.

Tutorials: The tutorial hour will be utilized for an overall review of the topics covered in the lectures, and problem-solving. Similar to the problems discussed/solved in the tutorial may be included in the evaluation. In addition, a part of the continuous evaluation will also be conducted during the tutorial hour.

Problem Sets: Several problem sets may be provided to the students. Additionally, it is expected from all the students to solve all of the problems given in the textbook and reference books independently, students may confer with their classmates or with the instructors. However, you need to write up the solutions to the problems on your own.

Evaluation Scheme:

Component	Duration (min)	Weightage (%)	Date and Time	Nature of Component
Mid-sem	90	30	05/11 9.00 - 10.30AM	Closed Book
Assignment & Class Tests	-	30	Continuous	Open Book
Comprehensive Examination	180	40	30/12 FN	Closed Book

*As per the timetable, **Dates will be announced at a later stage. Surprise tests may be conducted at any stage.

Attendance policy: It is expected from all the students to attend all scheduled lectures. Students are responsible for the topics covered in the lectures as well as worksheets, assignments, and take-home problem sets distributed during lectures.

Chamber consultation hour: Consultation hour will be announced later in the class/CMS.

e-mail of the instructor-in-Charge: m.dixit@hyderabad.bits-pilani.ac.in

Make-up policy: For genuine cases only.

Notices concerning the course will be displayed in **CMS**.

Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

Instructor-in-Charge
CHEM F213

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