Birla Institute of Technology & Science, Pilani
Hyderabad Campus

FIRST SEMESTER 2023-2024
Course Handout Part II

Date: 11/08/2023

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 : **K. Sumithra**

Scope and Objectives: The principles of quantum mechanics will be introduced, and application to problems in electronic structure of atoms, chemical bonding and spectroscopy will be discussed.

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).

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** MathChapter 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.

Evaluation Scheme:

Component	Duration (min)	Weightage (%)	Date and Time	Nature of Component
Mid-sem	90	30	11/10 9.30 - 11.00AM	Closed Book
Assignment / Class Tests	-	30	Continuous	Open Book
Comprehensive Examination	180	40	12/12 FN	Closed Book

Note: Active and regular participation in the class discussions is expected from each student. **The students are expected to work with mathematica to plot the polar plots and radial functions of the hydrogenic orbitals.**

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