Birla Institute of Technology & Science, Pilani
Hyderabad Campus

FIRST SEMESTER 2020-2021
<u>Course Handout Part II</u>

Date: 17/08/2020

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

Course No. : **CHEM F213**
Course Title : **Physical Chemistry-II**
Instructor-in charge : **K. Sumithra**

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

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*	*Learning Objectives*	*Ref. to text*
	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.	1.1-1.10
3	Wave-Particle Duality	De Broglie's postulate, Heisenberg Uncertainty Principle	1.11-1.14
4-5	The Wave Equation	Normal modes, superposition, Fourier series	2.1-2.5
6-8	Postulates of Quantum Mechanics	Wave function,, Operators and Observables, Schrodinger equation, Time Evolution and Stationary States, Uncertainty	3.1-3.4, 3.7,8,11, 4.1-4.9
	Some Exactly Solvable Problems		
9-10	Particle in a Box	Bound States, Zero Point Energy, Symmetry, Superposition States, Degeneracy in 2 and 3 dimensions	3.4-3.11, 6.1-6.2
11-12	Finite Potential Wells and Barriers	Bound States in Wells, Probability Current, Reflection and Tunneling	Class Notes, Ref (b) 12.3
13-15	Harmonic Oscillator	Eigenstates, Molecular Vibration	5.1-5.13

16-18	Angular Momentum and Rigid Rotator	Energy levels, Commutation Relations and Wavefunctions, Molecular Rotation	6.3-6.7, 6.10
19-20	The Hydrogen atom	Energy levels, Wavefunctions – Angular and Radial Parts, Orbitals	6.8-6.11
	Approximation Methods		
21-23	Variation Method	Variation theorem, application including Linear Variation	6.12, 7.3-7.7, 8.1,2
24-25	Stationary State Perturbation Theory	Systematic Correction of Wavefunctions and Energies, Treatment of Degenerate States	7.1,2, 8.2 Ref (a) 9.1-7
	Many Electron Atoms		
26-27	Many Electron Wavefunctions	Systems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants	8.4-6
28	SCF Method	Hartree and Hartree-Fock Methods, Periodicity	8.3,7,8
29-30	Atomic Terms and Spectra	Addition of Angular Momenta, Spin-Orbit Interaction, Selection Rules	8.9-8.12
	Molecules		
31	Born-Oppenheimer Approximation	Separation of nuclear and electronic motion	9.1
32-33	Valence Bond Theory – H_2	Localized Electron Pair Bonds	9.2-9.5
34-35	Molecular Orbital Theory – H_2^+, H_2	Linear Combination of Atomic Orbitals, Comparison to VB Picture	9.6-9.8
36-37	Homonuclear Diatomic Molecules	Molecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms	9.9-9.15
38-39	Hückel MO theory	π-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders	9.21-9.24
40-42	Molecular Spectroscopy	Vibration-Rotation Spectra, Selection Rules, Electronic Spectra and the Franck-Condon Principle	10.1-10.18

Expected Learning outcomes:

Lectures	*Learning outcome*
1-2	Relate 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 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 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	Recognize theoretical concepts behind electronic structure calculations of polyatomic molecules
29-30	Examine the allowed and forbidden transition in atoms

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

Evaluation Scheme:

Component	**Duration (min)**	**Weightage (%)**	**Date and Time**	**Remarks**
Test I	30	10	September 10 – September 20 (During scheduled class hour)	Open Book
Test II	30	15	October 09 –October 20 (During scheduled class hour)	Open Book
Test III	30	15	November 10 – November 20 (During scheduled class hour)	Open book
Assignment/Quiz/Viva	-	25	continuous	Open book
Comprehensive Examination	120	35	TBA	Open book

Note: Active and regular participation in the online class discussions is expected from each student.

Chamber consultation hour: Consultation can be done via e-mail.

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