# FIRST SEMESTER 2019-2020 Course Handout (Part II)

01/08/2019

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, 5<sup>th</sup> ed., PHI (2008).
- (b) Physical Chemistry', P W Atkins & Julio de Paula, 8<sup>th</sup> ed., OUP (2006).
- (c) 'Introduction to Quantum Mechanics with applications to Chemistry', Linus Pauling and E. Bright Wilson, Jr., Dover (1962)

## **Course Plan:**

Lect.	Topics	Learning Objectives	Ref. to text		
No.	_		-		
	Development of Quantum Theory				
1-2	Origins of Quantum	Blackbody Radiation, Photoelectric Effect, Atomic	1.1-1.10		
	Theory	Vibration in Crystals, Line Spectra & Bohr Model of H Atom.			
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	Wave function,, Operators and Observables, Schrodinger	3.1-3.4,		
	Quantum	equation, Time Evolution and Stationary States,	3.7,8,11,		
	Mechanics	Uncertainty	4.1-4.9		
	Some Exactly Solval	ole Problems			
9-10	Particle in a Box	Bound States, Zero Point Energy, Symmetry,	3.4-3.11,		
		Superposition States, Degeneracy in 2 and 3 dimensions	6.1-6.2		
11-12	Finite Potential	Bound States in Wells, Probability Current, Reflection and	Class		
	Wells and Barriers	Tunneling	Notes, Ref		
			(b) 12.3		
13-15	Harmonic Oscillator	Eigenstates, Molecular Vibration	5.1-5.13		

16-18 18-18 19-20Angular Momentum and Rigid Rotator The Hydrogen atomEnergy levels, Commutation Relations and Wavefunctions, Molecular Rotation Energy levels, Wavefunctions – Angular and Radial Parts, Orbitals6.36-6.71Approximation Methods21-23Variation Method Perturbation TheoryVariation theorem, application including Linear Variation Treatment of Degenerate States6.12, 7.3-7.7, 8.1,224-25 Perturbation TheorySystematic Correction of Wavefunctions and Energies, Treatment of Degenerate States7Many Electron AtomsSystems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants8.4-628 29-30 Atomic Terms and SpectraAddition of Angular Momenta, Spin-Orbit Interaction, Selection Rules8.9-8.1231 32-33 40-35 Theory – H₂', H₂ Diatomic MoleculesSeparation of nuclear and electronic motion VB Picture9.136-37 Diatomic MoleculesLinear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.838-39 40-42 Molecular Molecular Molecular Molecular Molecular Molecular Electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders9.21-9.2440-42 Molecular Molecular Molecular Molecular SpectroscopyMolecular Franck-Condon Principle10.1-10.18		1				
The Hydrogen atom Privation Surprivation Privates (Privation Method)       Energy levels, Wavefunctions – Angular and Radial Parts, Orbitals       6.8-6.11         21-23       Approximation Method       Variation theorem, application including Linear Variation       6.12, 7.3-7.8.1,2         24-25       Stationary State Perturbation Theory       Systematic Correction of Wavefunctions and Energies, Treatment of Degenerate States       7.1,2, 8.2         Perturbation Theory       Treatment of Degenerate States       8.46 (a) 9.1-7         26-27       Many Electron Atomic Terms and 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         31       Born-Oppenheimer Approximation       Separation of nuclear and electronic motion       9.1         32-33       Valence Bond Theory − H₂       Linear Combination of Atomic Orbitals, Comparison to VB Picture       9.6-9.8         34-35       Molecular Orbital Theory − H₂*, H₂       Molecular Electronic Configuration, SCF-LCAO-MO       9.9-9.15         36-37       Homonuclear Diatomic Molecular Electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders       9.21-9.24         40-42       Molecular <td>16-18</td> <td>Angular Momentum</td> <td>Energy levels, Commutation Relations and</td> <td>6.3-6.7,</td>	16-18	Angular Momentum	Energy levels, Commutation Relations and	6.3-6.7,		
Approximation Methods         21-23       Variation Method       Variation theorem, application including Linear Variation       6.12, 7.3-7, 8.1,2         24-25       Stationary State Perturbation Theory       Systematic Correction of Wavefunctions and Energies, To,2, 8.2 Ref (a) 9.1-7       7.1,2, 8.2 Ref (a) 9.1-7         Many Electron Atoms         26-27       Many Electron Systems of Identical Particles, Spin & Permutation Wavefunctions       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         31       Born-Oppenheimer Approximation       Separation of nuclear and electronic motion       9.1         32-33       Valence Bond Theory − H₂       Localized Electron Pair Bonds       9.2-9.5         34-35       Molecular Orbital Theory − H₂*, H₂       Linear Combination of Atomic Orbitals, Comparison to VB Picture       9.9-9.15         36-37       Homonuclear Diatomic Molecules       Molecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms       9.9-9.15         38-39       Hückel MO theory Arcelectron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders       9.21-9.24         40-42       Molecular       Vibration-Rotation Spec		and Rigid Rotator	Wavefunctions, Molecular Rotation	6.10		
Approximation Methods21-23Variation MethodVariation theorem, application including Linear Variation6.12, 7.3-7.7, 8.1,224-25Stationary State Perturbation TheorySystematic Correction of Wavefunctions and Energies, Treatment of Degenerate States7.1,2, 8.2 Ref (a) 9.1-7Many Electron Atoms26-27Many ElectronSystems of Identical Particles, Spin & Permutation Wavefunctions8.4-628SCF MethodHartree and Hartree-Fock Methods, Periodicity8.3,7,829-30Atomic Terms and SpectraAddition of Angular Momenta, Spin-Orbit Interaction, Selection Rules8.9-8.1231Born-Oppenheimer ApproximationSeparation of nuclear and electronic motion9.132-33Valence Bond Theory – H2Localized Electron Pair Bonds9.2-9.534-35Molecular Orbital Theory – H2*, H2Linear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.836-37Homonuclear Diatomic MoleculesMolecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms9.9-9.1538-39Hückel MO theory Hückel MO theoryπ-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18	19-20	The Hydrogen atom	Energy levels, Wavefunctions – Angular and Radial Parts,	6.8-6.11		
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24-25 Stationary State Perturbation Theory Many Electron Atoms  26-27 Many Electron Wavefunctions  28 SCF Method Systems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants  29-30 Atomic Terms and Spectra Selection Rules  31 Born-Oppenheimer Approximation 32-33 Valence Bond Theory – H <sub>2</sub> Theory – H <sub>2</sub> Theory – H <sub>2</sub> 34-35 Molecular Orbital Theory – H <sub>2</sub> Theory – H <sub>2</sub> 36-37 Homonuclear Diatomic Molecules  38-39 Hückel MO theory Hückel MO theory  Treatment of Degenerate States  Systems of Identical Particles, Spin & Permutation Systems of Identical Particles, Spin & Permutation Systems of Identical Particles, Spin & Permutation Addition of Angular Momenta, Spin-Orbit Interaction, Spectra Selection Rules  Separation of nuclear and electronic motion  9.1  9.2-9.5  10 Separation of nuclear and electronic motion Spectra Selection Pair Bonds Theory – H <sub>2</sub>		Approximation Met	hods			
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28 SCF Method Hartree and Hartree-Fock Methods, Periodicity 8.3,7,8 29-30 Atomic Terms and Spectra Selection Rules  Molecules  31 Born-Oppenheimer Approximation 32-33 Valence Bond Theory – H2 34-35 Molecular Orbital Theory – H2+, H2 36-37 Homonuclear Diatomic Molecules  38-39 Hückel MO theory Tolera Molecular Policular Diatomic Molecular Terms  38-39 Hückel MO theory Tolera Tolera Molecular Policular Spectra, Selection Rules, Electronic 10.1-10.18	26-27	Many Electron	Systems of Identical Particles, Spin & Permutation	8.4-6		
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Molecules31Born-Oppenheimer ApproximationSeparation of nuclear and electronic motion9.132-33Valence Bond Theory – H2Localized Electron Pair Bonds9.2-9.534-35Molecular Orbital Theory – H2+, H2Linear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.836-37Homonuclear Molecular Electronic Configuration, SCF-LCAO-MO Diatomic Molecules9.9-9.1538-39Hückel MO theory Ar-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18	29-30	Atomic Terms and	Addition of Angular Momenta, Spin-Orbit Interaction,	8.9-8.12		
31Born-Oppenheimer ApproximationSeparation of nuclear and electronic motion9.132-33Valence Bond Theory – H2Localized Electron Pair Bonds9.2-9.534-35Molecular Orbital Theory – H2+, H2Linear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.836-37Homonuclear Diatomic MoleculesMolecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms9.9-9.1538-39Hückel MO theory and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18			Selection Rules			
Approximation  32-33 Valence Bond Localized Electron Pair Bonds  Theory – H <sub>2</sub> 34-35 Molecular Orbital Theory – H <sub>2</sub> Theory – H <sub>2</sub> <sup>+</sup> , H <sub>2</sub> VB Picture  36-37 Homonuclear Diatomic Molecules  Wavefunctions, Molecular Terms  38-39 Hückel MO theory π-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders  40-42 Molecular  Valence Bond 9.2-9.5  Verall Combination of Atomic Orbitals, Comparison to 9.6-9.8  VB Picture  VB Picture  Molecular Electronic Configuration, SCF-LCAO-MO 9.9-9.15  Wavefunctions, Molecular Terms  7-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders  40-42 Molecular  Vibration-Rotation Spectra, Selection Rules, Electronic		Molecules				
32-33Valence Bond Theory – H2Localized Electron Pair Bonds9.2-9.534-35Molecular Orbital Theory – H2+, H2Linear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.836-37Homonuclear Diatomic MoleculesMolecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms9.9-9.1538-39Hückel MO theory and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18	31	Born-Oppenheimer	Separation of nuclear and electronic motion	9.1		
Theory – H2Linear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.836-37Homonuclear Diatomic MoleculesMolecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms9.9-9.1538-39Hückel MO theory and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18		Approximation				
34-35Molecular Orbital Theory – H2+, H2Linear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.836-37Homonuclear Diatomic MoleculesMolecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms9.9-9.1538-39Hückel MO theory and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18	32-33	Valence Bond	Localized Electron Pair Bonds	9.2-9.5		
Theory – H <sub>2</sub> <sup>+</sup> , H <sub>2</sub> VB Picture  36-37 Homonuclear Molecular Electronic Configuration, SCF-LCAO-MO Diatomic Molecules Wavefunctions, Molecular Terms  38-39 Hückel MO theory π-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders  40-42 Molecular Vibration-Rotation Spectra, Selection Rules, Electronic 10.1-10.18						
36-37Homonuclear Diatomic MoleculesMolecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms9.9-9.1538-39Hückel MO theory and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18	34-35	Molecular Orbital	Linear Combination of Atomic Orbitals, Comparison to	9.6-9.8		
Diatomic MoleculesWavefunctions, Molecular Terms38-39Hückel MO theoryπ-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18		Theory $-H_2^+$ , $H_2$	VB Picture			
38-39Hückel MO theory and delocalization, charge distribution and bond ordersπ-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18	36-37			9.9-9.15		
and delocalization, charge distribution and bond orders  40-42 Molecular Vibration-Rotation Spectra, Selection Rules, Electronic 10.1-10.18						
40-42 Molecular Vibration-Rotation Spectra, Selection Rules, Electronic 10.1-10.18	38-39	Hückel MO theory		9.21-9.24		
<u> </u>						
Spectroscopy Spectra and the Franck-Condon Principle	40-42	Molecular	Vibration-Rotation Spectra, Selection Rules, Electronic	10.1-10.18		
		Spectroscopy	Spectra and the Franck-Condon Principle			

# **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	Weightage (%)	Date & Time	Remarks
Assignments		15	Continuous	Open book
Seminar/Interaction/Take home		5	Continuous	Open book
Assignment				
Mid-semester Test	90 min.	35	3/10, 11.00 12.30 PM	Closed book
Comprehensive Examination	3 hrs.	45	09/12 AN	Closed book

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

**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.

Make-up policy: for genuine cases only

**Chamber consultation hour**: Monday 4-5 pm and any other time with prior appointment.

**Notices** concerning the course will be displayed on the **Chemistry Department Notice Board and/or in CMS**.

Instructor-in-Charge CHEM F213

