FIRST SEMESTER 2020-2021 Course Handout Part II

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.	Topics	Learning Objectives	Ref. to text			
No.	D 1					
	Development of Qua	ment 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	De Broglie's postulate, Heisenberg Uncertainty Principle	1.11-1.14			
	Duality					
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 States7.1,2, 8.2Many 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 32-31 ApproximationSeparation of nuclear and electronic motion9.132-33 Avalence Bond Theory – H2 H2 Homonuclear Diatomic MoleculesLinear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.836-37 Bickel MO theory Diatomic MoleculesMolecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms9.21-9.2438-39 Bickel MO theory Molecular Spectroscopyπ-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders9.21-9.2440-42 BopectroscopyMolecular Spectra and the 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 StateSystematic Correction of Wavefunctions and Energies, Treatment of Degenerate States7.1,2, 8.2Perturbation TheoryTreatment of Degenerate StatesRef (a) 9.1-7Many Electron Atoms26-27Many ElectronSystems of Identical Particles, Spin & Permutation8.4-6WavefunctionsSymmetry, Pauli Principle, Slater Determinants8.9-8.1229-30Atomic 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 Theory - H2*, H2VB Picture36-37Homonuclear Molecular Molecular Electronic Configuration, SCF-LCAO-MO Diatomic Molecular9.9-9.1538-39Hückel MO theory	19-20	The Hydrogen atom	Energy levels, Wavefunctions – Angular and Radial Parts,	6.8-6.11
21-23Variation Method Stationary State Perturbation TheoryVariation theorem, application including Linear Variation 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 AtomsTreatment of Degenerate StatesRef (a) 9.1-726-27Many Electron WavefunctionsSystems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants8.4-628SCF Method SpectraHartree and Hartree-Fock Methods, Periodicity Selection Rules8.9-8.1229-30Atomic Terms and SpectraSelection 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 Picture9.6-9.836-37Monuclear 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			Orbitals	
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 ₂ Theory – H ₂ Theory – H ₂ 34-35 Molecular Orbital Theory – H ₂ Theory – H ₂ 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 ₂		Approximation Met	hods	
24-25Stationary State Perturbation TheorySystematic Correction of Wavefunctions and Energies, Treatment of Degenerate States7.1,2,8.2 Ref (a) 9.1-7Many Electron Atoms26-27Many Electron WavefunctionsSystems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants8.4-628SCF Method Symmetry, Pauli Principle, Slater Determinants8.3,7,829-30Atomic 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 Bonds Theory – H2*, H29.2-9.534-35Molecular 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			Variation theorem, application including Linear Variation	6.12, 7.3-
Perturbation TheoryTreatment of Degenerate StatesRef (a) 9.1-7Many Electron Atoms26-27Many Electron WavefunctionsSystems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants8.4-628SCF 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 – H₂², H₂Linear Combination of Atomic Orbitals, Comparison to VB Picture9.6-9.836-37Homonuclear Diatomic MoleculesMolecular Electronic Configuration, SCF-LCAO-MO9.9-9.1538-39Hückel MO theory Theory – H₂² Arelectron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18				7.7, 8.1,2
Many Electron Atoms726-27Many Electron WavefunctionsSystems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants8.4-628SCF 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 MoleculesMolecular Electronic Configuration, SCF-LCAO-MO Diatomic Molecules9.9-9.1538-39Hückel MO theory A-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	24-25	Stationary State	Systematic Correction of Wavefunctions and Energies,	7.1,2, 8.2
Many Electron Atoms26-27Many Electron WavefunctionsSystems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants8.4-628SCF Method Atomic Terms and SpectraHartree and Hartree-Fock Methods, Periodicity Selection Rules8.9-8.1231Born-Oppenheimer ApproximationSelection Rules8.9-8.1232-33Valence Bond Theory – H2Separation of nuclear and electronic motion Theory – H2*9.2-9.534-35Molecular 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 theory An-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		Perturbation Theory	Treatment of Degenerate States	Ref (a) 9.1-
26-27Many Electron WavefunctionsSystems of Identical Particles, Spin & Permutation Symmetry, Pauli Principle, Slater Determinants8.4-628SCF 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 theory An 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				
WavefunctionsSymmetry, Pauli Principle, Slater Determinants28SCF MethodHartree and Hartree-Fock Methods, Periodicity8.3,7,829-30Atomic Terms and SpectraAddition of Angular Momenta, Spin-Orbit Interaction, Selection Rules8.9-8.12Molecules31Born-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 theory and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18		Many Electron Aton	ns	
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
29-30Atomic Terms and SpectraAddition of Angular Momenta, Spin-Orbit Interaction, Selection Rules8.9-8.12Molecules31Born-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 theory and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18		Wavefunctions	Symmetry, Pauli Principle, Slater Determinants	
29-30Atomic Terms and SpectraAddition of Angular Momenta, Spin-Orbit Interaction, Selection Rules8.9-8.12Molecules31Born-Oppenheimer ApproximationSeparation of nuclear and electronic motion9.132-33Valence Bond Theory – H₂Localized Electron Pair Bonds9.2-9.534-35Molecular Orbital Theory – H₂²⁺, 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 theory and delocalization, charge distribution and bond orders9.21-9.2440-42MolecularVibration-Rotation Spectra, Selection Rules, Electronic10.1-10.18				
29-30Atomic Terms and SpectraAddition of Angular Momenta, Spin-Orbit Interaction, Selection Rules8.9-8.12Molecules31Born-Oppenheimer ApproximationSeparation of nuclear and electronic motion9.132-33Valence Bond Theory – H₂Localized Electron Pair Bonds9.2-9.534-35Molecular Orbital Theory – H₂²⁺, 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 theory A-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				
SpectraSelection RulesMolecules31Born-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 Au-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	28	SCF Method	Hartree and Hartree-Fock Methods, Periodicity	8.3,7,8
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		Spectra Selection Rules		
Approximation 32-33 Valence Bond Localized Electron Pair Bonds Theory – H ₂ 34-35 Molecular Orbital Theory – H ₂ Theory – H ₂ ⁺ , H ₂ 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 ₂ ⁺ , H ₂ 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 and Time	Remarks
	(min)	(%)		
Test I	30	10	September 10 –	Open Book
			September 20 (During	
			scheduled class hour)	
Test II	30	15	October 09 –October 20	Open Book
			(During scheduled class	
			hour)	
Test III	30	15	November 10 –	Open book
			November 20 (During	
			scheduled class hour)	
Assignment/Quiz/Viva	-	25	continuous	Open book
Comprehensive	120	35	TBA	Open book
Examination				

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

