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**FIRST SEMESTER 2021-2022**

**Course Handout Part II**

Date: 20/08/2021

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:**

1. ‘Quantum Chemistry’, Ira N Levine, 5th ed., PHI (2008).
2. Physical Chemistry’, P W Atkins & Julio de Paula, 8th ed., OUP (2006).
3. ‘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. | 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 | Atomic Terms and Spectra | Addition of Angular Momenta (S.S), Spin-Orbit Interaction (S.S), Selection Rules | 8.9-8.12 |
|  | **Molecules** | |  |
| 29 | Born-Oppenheimer Approximation | Separation of nuclear and electronic motion | 9.1 |
| 30-31 | Valence Bond Theory – H2 | Localized Electron Pair Bonds | 9.2-9.5 |
| 32-33 | Molecular Orbital Theory – H2+, H2 | Linear Combination of Atomic Orbitals, Comparison to VB Picture | 9.6-9.8 |
| 34-35 | Homonuclear Diatomic Molecules | Molecular Electronic Configuration, SCF-LCAO-MO Wavefunctions, Molecular Terms | 9.9-9.15 |
| 36-37 | Hückel MO theory | -electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders | 9.21-9.24 |
| 38-40 | Molecular Spectroscopy | Vibration-Rotation Spectra, Selection Rules, Electronic Spectra and the Franck-Condon Principle | 10.1-10.18 |

**Expected Learning outcomes:**

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| --- | --- |
| *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 | Examine the allowed and forbidden transition in atoms |
| 29 | Express molecular wavefunction as 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:**

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| --- | --- | --- | --- | --- |
| **Component** | **Duration**  **(min)** | **Weightage (%)** | **Date and Time** | **Nature of Component** |
| Midsem | 90 | 30 | 22/10/2021 9.00 - 10.30AM | Open book |
| Assignment/Class Tests | - | 30 | continuous | Open book |
| Comprehensive Examination | 120 | 40 | 22/12 AN | Closed book |

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

**Chamber consultation hour:** To be announced through a notice.

**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

