First SEMESTER 2018 - 2019
Course Handout (Part II)

Date: 02.08.2018

In addition to part I (General Handout for all courses appended to the time table) this portion gives further specific details with regard to this course.

Course No. : **CHEM F213**
Course Title : **Physical Chemistry - II**
Instructor-in-charge : **Prashant Uday Manohar**

Objective of the course: The course provides an introduction to quantum mechanics and application of quantum mechanics to electronic structure of atoms / molecules, chemical bonding, and spectroscopy.

Text Book (TB): Quantum Chemistry, Donald A McQuarrie, University Science Books (First Indian Edition 2003, Viva Books Private Limited)

Reference Books (RB):
RB-1: *Quantum Chemistry*, Ira N. Levine, 7th Edition, PHI, 2014,
RB-2: *Quantum Mechanics*, Bransden and Joachain, 2nd Edition, Pearson.
RB-3: *Atkins' Physical Chemistry*, 9th Edition, Peter Atkins and Julio De Paula, Oxford University Press.
RB-4: *Introduction to Quantum Mechanics with Applications to Chemistry*, Linus Pauling and E. Bright Wilson, Jr., Dover Publications, Inc, New York.
RB-5: *Elements of Quantum Mechanics*, Michael D. Fayer, Oxford University Press, New York, 2001.

Course Plan:

Module – 01: Development of Quantum Theory: Lecture – 01 (L-01) to Lecture – 08 (L-08)

- **L-01 to L-02: Failure of classical physics and origin of quantum theory.**
  - Learning objectives: Blackbody radiation, Photoelectric Effect, Atomic Vibrations in Crystals, Line Spectra and Bohr Model of H Atom, de Broglie's postulate, Heisenberg uncertainty principle.
  - Learning outcome: Recognize the necessity of quantum theory.
  - Reference: TB, 1.1 – 1.4
- **L-03: The wave equation**
  - Learning objectives: Motion of vibrating string, separation of variables, normal modes, superposition, Fourier series.
  - Learning outcome: Recognize mathematical background for quantum theory.
  - Reference: TB, 2.1 – 2.5
- **L-04 to L-08: Postulates of quantum mechanics**
  - Learning objectives: Wave function, Schrödinger equation, operators and observables, eigenvalue problem, time evaluation and stationary states, uncertainty, measurement and superposition of states.
  - Learning outcome: Consolidate new concepts to be used in quantum mechanics
  - Reference: TB, 3.1 – 3.4, 3.7, 3.8, 3.11, 4.1 – 4.9; RB-2, 7.1 – 7.10

Module – 02: Some exactly solvable problems: L-09 to L-20

- **L-09 to L-10: Particle in a Box (PIB)**
  - Learning objectives: Bound states, Zero point energy, symmetry, superposition states, and degeneracy in two- and three-dimensions.
  - Learning outcome: Theorize quantization of states and zero point energy in very simple systems, like, PIB.
  - Reference: TB, 3.4 – 3.11, 6.1 – 6.2
- **L-11 to L-12: Finite potential wells and barriers**
  - Learning objectives: Bound states in wells, probability current, reflections and tunneling.
  - Learning outcome: Recognize working principle of scanning tunneling microscopy.
  - Reference: Study materials; RB-2, 2.5; RB-3, 8.3
- **L-13 to L-15: Harmonic oscillator**

- Learning objectives: Eigen states for simple harmonic oscillator, zero point energy, molecular vibration, dissociation energy, and anharmonicity.
- Learning outcome: Define vibrational spectroscopy of molecules.
- Reference: TB, 5.1 – 5.13

➢ **L-16 to L-18: Angular momentum and rigid rotor**
- Learning objectives: Energy levels, operator for angular momentum, commutation relation, wavefunction, and molecular rotation.
- Learning outcome: Define rigid rotator as model for rotating diatomic molecules.
- Reference: TB, 6.3 – 6.7, 6.10

➢ **L-19 to L-20: The hydrogen atom**
- Learning objectives:Energy levels, wavefunction – angular and radial parts, orbitals, and effect of magnetic field on hydrogen atom.
- Learning outcome:Review atomic orbital picture of H-atom from quantum mechanics.
- Reference: 6.8 – 6.11

Module – 03: Approximation methods: L-21 to L-25

➢ **L-21 to L-23: Variation method**
- Learning objectives: Schrödinger equation for He-atom cannot be solved exactly, variation theorem, linear variation method.
- Learning outcome: Evaluate the upper bound to the ground state energy of a system.
- Reference: 6.12, 7.3 – 7.7, 8.1, 8.2

➢ **L-24 to L-25: Perturbation theory for stationary state**
- Learning objectives: Systematic correction of wavefunction and energies of non-degenerate states.
- Learning outcome: Calculate ground state energy of various systems from the unperturbed state of the system.
- Reference: TB, 7,1, 7.2, 8.2; RB-2, 9.1 – 9.7

Module – 04: Many electron atoms: L-26 to L-30

➢ **L-26: Many electron wavefunction**
- Learning objectives: Systems of identical particles, spin and permutation symmetry, Pauli principle, and Slater determinants.
- Learning outcome: Define spin as another coordinate.
- Reference: TB, 8.4 – 8.6

➢ **L-27 to L-29: SCF method**
- Learning objectives: Hartree and Hartree-Fock methods, electronic structure calculations, comparison with experimental data, periodicity.
- Learning outcome: Recognize theoretical concepts behind electronic structure calculations of polyatomic molecules.
- Reference: TB, 8.3, 8.7, 8.8

➢ **L-30: Atomic terms and spectra**
- Learning objectives: Addition of angular momenta, spin-orbit interaction, absorption and emission spectra of atoms, selection rules.
- Learning outcome: Examine allowed and forbidden transition in atoms.
- Reference: TB, 8.9 – 8.12

Module – 05: Molecules: L-31 to L-38

➢ **L-31: Born-Oppenheimer approximation**
- Learning objectives: Separation of nuclear and electronic motion.
- Learning outcome: Express molecular wavefunction as product of nuclear and electronic wavefunctions.
- Reference: TB, 9.1

➢ **L-32 to L-33: Valence Bond Theory – H_2**
- Learning objectives: Localized electron pair bonds.
- Learning outcome: Demonstrate successful description of chemical bond.
- Reference: TB, 9.2 – 9.5

➢ **L-34 to L-35: Molecular Orbital Theory – H_2^+, H_2**
- Learning objectives: Linear combination of atomic orbitals, comparison to valence bond picture.
- Learning outcome: Illustrate application of molecular orbital theory to diatomic molecules.
- Reference: 9.6 – 9.8

➢ **L-36 to L-37: Homonuclear diatomic molecules**
- Learning objectives: Molecular electronic configuration, Pauli principle, SCF-LCAO-MO wavefuncitons, and molecular terms.
- Learning outcome: Compare experimental observations along with theoretical prediction for diatomic molecules.

- Reference: TB, 9.9 – 1.5
- **L-38: Hückel MO theory**
  - Learning objectives: π-electron approximation for conjugated systems, energies and delocalization, atomic charge distribution and bond order.
  - Learning outcome: Explore quantum chemical approximation of aromatic systems.
  - Reference: TB, 9.21 – 9.24

Module – 06: Molecular spectroscopy: L-39 to L-42

- **L-39: Electromagnetic radiation and its interaction with molecules**
  - Learning objectives: Perturbation theory of degenerate energy levels, time dependent perturbation theory, interaction of radiation and matter, absorption, emission.
  - Learning outcome: Recognize quantum-mechanical approach for spectroscopy.
  - Reference: RB-2, 9.5, 9.9, 9.10
- **L-40: Rotational and vibrational spectra**
  - Learning objectives: Different regions of electromagnetic spectrum, molecular rotation, molecular vibration, normal modes, rotational transitions accompany vibrational transitions, Boltzman population distribution.
  - Learning outcome: Explain rotational and vibrational spectroscopy.
  - Reference: TB, 10.1 – 10.10; study material
- **L-41: Electronic spectra**
  - Learning objectives: Electronic states, transitions, vibrational and rotational information, intensity pattern.
  - Learning outcome: Recognize fundamentals of electronic spectroscopy.
  - Reference: TB, 10.11 – 10.13, study material
- **L-42: Selection rules and Franck-Condon principle**
  - Learning objectives: Overlap integrals, nuclear motion can be factored approximately into a rotational part and vibrational part, selection rule in rigid rotor, selection rule in harmonic oscillator, selection rule in electronic spectroscopy.
  - Learning outcome: Formulate allowed and forbidden transition.
  - Reference: 10.14 – 10.18

Learning outcome of the course:

1. Demonstrate the need of quantum mechanics to explain atomic and molecular phenomenon.
2. Apply concepts of quantum mechanics to simple and exactly solvable physical systems.
3. Explain bonding theories and their application to simple molecular systems.
4. Illustrate various approximation methods using quantum mechanics.
5. Formulate SCF methods for many electron system which is the basic of any electronic structure calculation for geometry optimization and energy calculation.
6. Application of quantum mechanics into molecular spectroscopy.

Tutorials hour: The tutorial hour will be utilized for review of the topics covered in the lectures, problem solving and for conducting a part of the continuous evaluation.

Continuous Evaluation: Continuous Evaluation will include the **evaluative components conducted during tutorial hour, take-home assignments, online assignments and interactive participation of students**. Solving problem sets is one of the efficient ways to explore-and-learn quantum chemistry. Students will be encouraged to discuss the problem sets among themselves and with the instructor-in-charge in addition to refer to books and internet. However, students are expected to solve the problems themselves and submit the same in their own handwriting on or before the deadline announced for each problem-set. Some evaluative assignments may be designed for online submission. Apart from this, interactive participation of students, such as in answering questions or in discussing a small portion of a topic, etc. during the lecture and tutorial hours will also be considered as a part of continuous evaluation.

Attendance policy: It is expected that students will attend all scheduled lectures. Students are responsible for the topics covered in the lectures as well as worksheets, assignment, and take home problem sets distributed during lectures and tutorials.

Evaluation Scheme:

Component	Duration	Weightage (%)	Date & Time
Mid Semester Test (Closed-book)	90 minutes	30	9/10 2:00 - 3:30 PM

*Continuous Evaluation (partly Open-book)		30	Continuous
Comprehensive Examination (partly Open-book)	180 minutes	40	3/12 FN

* Continuous evaluation would be comprised of various components as discussed earlier.

Consultation Hour: To be announced in the class

E-mail of the instructor: pumanohar@pilani.bits-pilani.ac.in

Notice: Notices concerning this course will be displayed on nalanda.bits-pilani.ac.in and/or on the Department of Chemistry Notice Board.

Make-up Policy: Refer to Part-I of the handout for details.

Instructor-in-charge
CHEM F213