BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI
INSTRUCTION DIVISION
FIRST SEMESTER 2016-2017
Course Handout (Part II)

Date: 1/8/2016

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**
Instructor : **G. Sundar**

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
38-40	Hückel MO theory	π-electron approximation for conjugated systems, energies and delocalization, charge distribution and bond orders	9.21-9.24
41-42	Molecular Spectroscopy	Vibration-Rotation Spectra, Selection Rules, Electronic Spectra and the Franck-Condon Principle	10.1-10.18

Evaluation Scheme:

Component	*Duration*	*Weightage (%)*	*Date & Time*	*Remarks*
Assignments *		20	Continuous	*
Test 1	60 min.	20	8/9/2016, 11:30-12:30 pm	CB
Test 2	60 min.	20	25/10/2016, 11:30-12:30 pm	CB
Comprehensive Examination	3 hrs.	40	7/12/2016 (AN)	CB

* Assignments will be evaluated continuously along with the lecture classes and averaged to 20% of total marks.

Note: Active and regular participation in the class room discussions is expected from each student.
Make-up policy : for genuine cases only
Chamber consultation hour: Monday 11am -12 pm
Notices concerning the course will be displayed on the **Chemistry Department Notice Board and CMS**.

Instructor-in-Charge
CHEM F213