BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

INSTRUCTION DIVISION

Second SEMESTER 2015-2016

Course Handout (Part II)

Date: 05.01.2016

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

Course No.	**: CHEM F244**
Course Title	**: Physical Chemistry III**
Instructor-in-charge	**: SHAMIK CHAKRABORTY**
Team of Instructors	**: Prashant Uday Manohar**

Scope and objective of the course: This course is designed in continuation to the Physical chemistry courses I and II which are already been offered to the students. Physical Chemistry III course is composed of two parts. The first part provides a comprehensive survey of various approximation methods in quantum chemistry. In addition, basic concepts of molecular mechanics approach would be introduced as well. In the second portion, students would be exposed to the symmetry, principles of group theory, and its application in molecular spectroscopy.

Course Description: Symmetry: symmetry operations, point groups, reducible and irreducible representations, character tables, SALC, degeneracy, vibrational modes IR-Raman activity identification; stationary state perturbation theory; time dependent perturbation theory; virial and Hellmann-Feynmann theorems; polyatomic molecules: SCF MO treatment, basis sets, population analysis, molecular electrostatic potentials, configuration interaction, Moller Plesset perturbation theory; semi empirical methods-all valence electron methods: CNDO, INDO, NDDO; Density Functional Theory: Hohenberg-Kohn theorems, Kohn-Sham self consistent field approach, exchange correlation functional; molecular mechanics.

Text Book (TB): TB-1:"Quantum Chemistry", Ira N. Levine, PHI Learning Private Limited, Sixth Edition, 2012. **TB-2**: "Chemical Applications of Group Theory", F. Albert Cotton, Wiley Student Edition, Third Edition.

Reference Books (RB): Quantum Chemistry, Donald A McQuarrie, University Science Books (First Indian Edition 2003, Viva Books Private Limited)

Course Plan:

Lecture no.	Topic	Learning objectives	Reference to Text
	Electronic structure polyatomic molecules: (a) Theorems		
01-04	Theorems of molecular quantum mechanics	Virial theorem and Chemical Bonding, Hellmann-Feynman theorem, Electrostatic theorem	**TB-1** 14.1 – 14.7
	Electronic structure polyatomic molecules: (b) Molecular Orbital treatment		
SELF STUDY	Approximation Theorem of Many Electron Atoms	The Hartree SCF Method and Hartree-Fock SCF Method for many electron atoms	**RB 1**

05-08	Molecular electronic structure calculations	SCF-MO treatment, basis functions, population analysis, molecular electrostatic potential, localized MOs, SCF-MO treatment of H_2O	**TB-1** 13.15, 15.1 – 15.5, 15.6 – 15.9
09-11	Configuration Interaction	Configuration state functions, occupied and virtual molecular orbitals, excitation energy calculation.	**TB-1** 11.3, 16.1, class notes
12-14	Stationary state perturbation theory	Perturbation treatment of non-degenerate and degenerate states.	**TB-1** 9.1 – 9.7
15-17	Møller– Plesset Perturbation theory	Many body perturbation theory, electron correlation effects, Møller– Plesset perturbation of 2^{nd}, 3^{rd}, and 4^{th} order	**TB-1** 16.2
	Electronic structure polyatomic molecules: (c) Alternate approaches		
SELF STUDY	Valence-Bond approach	Coupling of electrons, bond eigenfunction, application of Valence-Bond treatment to different polyatomic molecules	**TB-1** 16.8
18-22	Density Functional Theory	Hohenberg-Kohn Theorem, Kohn-Sham method, exchange correlation functional, hybrid functional	**TB-1** 16.4, class notes
	Non-stationary states		
23-25	Time-dependent perturbation theory	Spectroscopy - interaction of electromagnetic radiation and matter	**TB-1** 9.9-9.10 Class Notes
	Molecular Symmetry and symmetry group		
26	Definitions and Theorems of Group Theory	Properties of a group, examples of groups, subgroups, classes	**TB-2** 2.1-2.4
27 - 28	Symmetry elements and operations	Plane, center of inversion, proper axis, and improper axis, product of symmetry operations, point groups	**TB-2** 3.1 – 3.9
29	Application of symmetry operations	Dipole moments, optical activity	**TB-2** 3.10 Class notes
30-31	Group Theory	Symmetry Point Group, Symmetry classification of molecules	**TB-2** 3.11 – 3.14
	Representation of Groups		
32-33	Equivalent and reducible representation	Unitary representation, reducible representation, transformation operators.	**TB-2** 4.2 – 4.5 Class notes
34-36	Irreducible representation	The "Great Orthogonality Theorem", characters, criterion for irreducibility, character tables and their construction	**TB-2** 4.2 – 4.5 Class notes
37-38	Representation and	Invariance of Hamiltonian operator under	**TB-2** 5.1 –

	quantum mechanics	transformation, direct product representation, vanishing integrals	5.3
39-40	Symmetry adapted linear combination (SALC)	Projection operators, construction of SALCs using projection operators.	**TB-2** 6.1 – 6.3
41-42	Molecular vibrations	Normal coordinates, vibrational levels, IR spectra, Raman spectra, selection rules.	**TB-2** 10.1 – 10.8

Evaluation Scheme: (Total 300 Marks)

Component	Duration (minutes)	Weightage (%)	Date and Time	Remarks
Continuous Evaluation[$]	-	35		Closed Book + Open book
Mid-semester	90	25	15/3 9:00 - 10:30 AM	Closed Book
Comprehensive Examination	180	40	5/5 FN	Closed Book + Open Book

[$] Assignment, Project, Class Test, Presentation

Chamber Consultation Hours: To be announced in class.

Notices: Notices, if any, concerning the course will be displayed on the Chemistry Department Notice Board.

Make up policy: Make up would be considered only for **genuine cases.**

Instructor in charge

CHEM F244