Birla Institute of Technology & Science, Pilani
Hyderabad Campus

SUMMER TERM-2022

Course Handout (Part - II)

Date: 5/28/2022

In addition to Part I (General Handout for all courses appended to the timetable), this portion gives further specific details regarding the course:

Course No. : CHEM F244
Course Title : Physical Chemistry III
Instructor-in-charge : **Mudit Dixit**

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

Scope and Objective: The principles of group theory, its application to molecular spectroscopy, and different approximate methods in quantum chemistry will be discussed. Basic concepts of density functional theory, semi-empirical methods, and molecular mechanics approach would also be introduced together with hands-on experiments on the application of these methods.

.

Text Book (T):
T: "Quantum Chemistry", Ira N. Levine, PHI Learning Private Limited, Sixth Edition, 2012.

Reference Books:
R1 : "Chemical Applications of Group Theory", F. Albert Cotton, Wiley Student Edition, Third Edition
R2. "Molecular symmetry and Group theory" Robert L Carter, Wiley (1998).

Course Plan:

Lec. No.	Learning Objectives	Topics to be covered	Chapter in the Text Book
Molecular Symmetry and Symmetry group			
1-3	Symmetry operations and Group theory	Symmetry elements, Point groups and their classification, Application of symmetry operations, dipole moment, and optical activity	T Chapter 12 R1 3.1 to 3.14, R2 1.5 to1.7
Representation of groups			

4-8	Equivalent and reducible representation, irreducible representation, and quantum mechanics	Irreducible and reducible representations, transformation operators, Great Orthogonality Theorem, Character tables, and their constructions, Hamiltonian operator under transformation, direct product representation, vanishing integrals	R1 4.2 to 4.5, R2 Chapter 2 (2.1 to 2.5) R1 5.1-5.3 Lecture notes
9-11	Symmetry and chemical bonding	Symmetry adapted linear combinations (SALCs), degeneracy, Projection operators	R1 6.1-6.3, R2 4.3, 5.1-5.2
12-14	Molecular vibrations	Normal coordinates, vibrational levels, IR spectra, Raman spectra, Selection Rules	R1 10.1-10.8 Lecture notes
15-16	Matrices	Matrix representation of operators	T 7.10, 8.6
Approximation Methods			
17-18	Variation Method	Recapitulation of the Variation theorem and method including Linear Variation	T 8.1 - 8.5
19-21 22-23	Stationary State Perturbation Theory Time-dependent perturbation theory	Recapitulation of perturbation theory, Systematic correction of energies and wave functions, non-degenerate and degenerate cases energy levels Spectroscopy-interaction of electromagnetic radiation and matter	T 9.1 - 9.7 T 9.9 - 9.10
Electronic structure calculation for polyatomic molecules			
24-28	Theorems of molecular quantum mechanics	Electron probability density, dipole moment, Hartree and Hartree-Fock method, Virial and Hellmann-Feynman theorems	T 14.1 - 14.6 T 11.3 Lecture notes
29-34	Molecular electronic structure calculations*	SCF MO Treatment, Basis Sets, Example of the water molecule, Population Analysis, MEP, Localized molecular orbitals Configuration Interaction, MP perturbation theory, Electron correlation methods.	Lecture notes T 15.1 - 15.6 T 15.7 - 15.9 T 16.1-16.2
35-36	Semi-empirical methods	Philosophy, π-electron methods (Huckel, EHM), examples all valence electron methods (CNDO, INDO, NDDO)	T 11.3,17.1, 17.4 Lecture notes
37-40	Density functional theory	Hohenberg-Kohn theorems, Kohn-Sham self-consistent field approach, exchange-correlation functional	T 16.4 Lecture notes
41-42	Molecular Mechanics	MM methods and their application	Lecture notes

Expected Learning outcomes:

Lectures	*Learning outcome*
1-3	Understand the elements of symmetry and point groups and apply these to chemical problems
4-8	Define and consolidate new concepts to be used in group theory
9-11	Understand and Apply the concepts of SALCs and Projection operators
12-14	Examine molecular vibrations and relate these to molecular spectroscopy
13-15	Define and interpret vibrational spectroscopy of molecules.
15-16	Define matrix representation of operators

17-18	Apply Variation Method for energy minimization process
19-21	Understand systematic correction of energies and wave functions through the Stationary State Perturbation Theory
22-23	Identify the spectroscopic interaction of electromagnetic radiation and matter
24-28	Understand and apply theorems of molecular quantum mechanics
29-34	Define the key elements of modern quantum chemical calculations
35-36	Understand the applicability of Semi-empirical methods define their limits and benefits
37-40	Explore the theoretical framework of density functional theory (DFT) and understand fundamental theorems related to DFT
41-42	Compare Molecular Mechanics with other computational methods and examine its applicability

Evaluation Scheme:

Component	**Weightage(%)**	**Duration**	**Date & Time**	**Nature of Component**
Continuous Evaluation*	30 (10% surprise tests (2) + 20% assignments (2))	During Class hrs	Continuous	Open book
Mid Sem Test	30	90 min.	25/06 3.30 - 5.00PM	Closed book
Comprehensive Examination	40	180 min.	22/07/2022 AN	Closed book

***It will be comprised of surprise tests /assignments.**

Chamber Consultation Hour: Will be announced later in the class and also will be displayed on the notice board.

Notices concerning the course will be displayed in CMS.

Make-up-policy: Make-up would be considered only for very genuine reasons.

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
Mudit Dixit