Birla Institute of Technology & Science, Pilani
Hyderabad Campus

SECOND SEMESTER 2019-2020

Course Handout (Part - II)

Date: 06/01/2020

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

Course No. : CHEM F244
Course Title : Physical Chemistry III
Instructor-in-charge : **K. Sumithra**

Scope and Objective: The principles of group theory, its application to molecular spectroscopy and different approximation 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.

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Text Book (T):
'Quantum Chemistry', Ira N Levine, 6th edition, Pearson Education Inc. (2009).

Reference Books:
R1."Chemical applications of Group theory" F. A. Cotton, Third Ed. Wiley (1990).
R2. "Molecular symmetry and Group theory" Robert L Carter, Wiley (1998).

Course Plan:

Lec. No.	Learning Objectives	Topics to be covered	Ref to text
Molecular Symmetry and Symmetry group			
1-3	Symmetry operations and Group theory	Symmetry elements, Point groups and its 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 adopted bases (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	7.10, 8.6
Approximation Methods			
17-18	Variation Method	Recapitulation of the Variation theorem and method including Linear Variation	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	9.1 - 9.7 9.9 - 9.10
Electronic structure calculation for polyatomic molecules			
24-28	Theorem of molecular quantum mechanics	Electron probability density, dipole moment, Hartree and Hatree-Fock method, Virial and Hellmann-Feynmann theorems	14.1 - 14.7 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	Lecture notes 15.1 - 15.6 15.7 - 15.9 16.1-16.2
35-36	Semi-empirical methods	Philosophy, π-electron methods (Huckel, PPP), all valence electron methods (CNDO, INDO, NDDO)	11.3,17.1 , 17.4 Lecture notes
37-38	Density functional theory	Hohenberg-Kohn theorems, Kohn-Sham self-consistent field approach, exchange correlation functional	16.4 Lecture notes
39-41	Molecular Mechanics	MM methods and its application	Lecture notes

Evaluation Scheme:

Component	Duration	Weightage(%)	Date & Time	Nature of Component
Continuous Evaluation*	During Class hr	25	Continuous	Open
Mid Sem Test	1.5 hrs	30	2/3 1.30 -3.00 PM	Closed book
Comprehensive	3 hrs	45	02/05 FN	Closed book

***It will be comprised of surprise tests and 4-5 mandatory computer experiments based on electronic structure calculations of polyatomic molecules.**

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

Notices concerning the course will be displayed only in the Chemistry Dept. Notice Board and 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
K. Sumithra