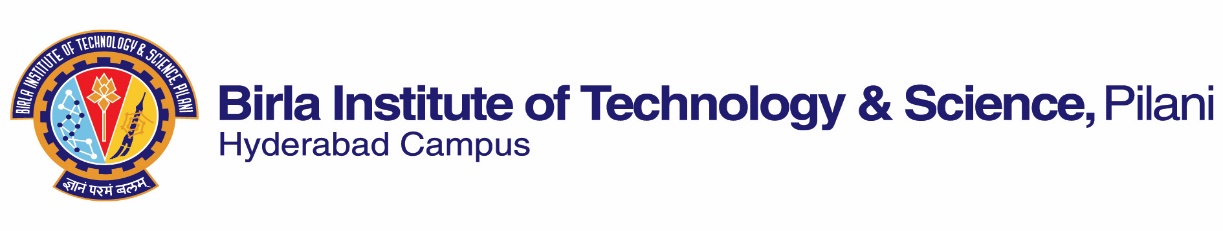
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**second SEMESTER 2022-2023**

**Course Handout (Part ‑ II)**

Date: 16/1/2023

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 F 244

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.

**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 | |
| 9-12 | | Symmetry and chemical bonding | Symmetry adopted bases (SALCs), degeneracy, Projection operators | R1 6.1-6.3,  R2 4.3, 5.1-5.2 | |
| 13-16 | | Molecular vibrations | Normal coordinates, vibrational levels, IR spectra, Raman spectra, Selection Rules | R1 10.1-10.8  Lecture notes | |
| 17-18 | | Matrices | Matrix representation of operators | 7.10, 8.6 | |
| **Approximation Methods** | | | | | |
| 19-20 | | Variation Method | Recapitulation of the Variation theorem and method including Linear Variation | 8.1 - 8.5 | |
| 21-23  24-25 | | 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** | | | | | |
| 25-30 | | Theorem of molecular quantum mechanics | Electron probability density, dipole moment, Hartree and Hatree-Fock method, Virial and Hellmann-Feynmann theorems | | 14.1 - 14.6  11.3  Lecture notes |
| 31-36 | | 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  15.1 - 15.6  15.7 - 15.9  16.1-16.2 |
| 37-39 | | Semi-empirical methods | Philosophy, π-electron methods (Huckel, EHM), examples all valence electron methods (CNDO, INDO, NDDO) | | 11.3,17.1 , 17.4 Lecture notes |
| 40-42 | | Molecular Mechanics | MM methods and its application | | Lecture notes |

**Evaluation Scheme**:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Component | Weightage(%) | Duration |  | Date & Time |
| Continuous Evaluation**\*** | 30 | During Class hrs | Open | Continuous |
| Mid Sem Test | 30 | 90 min. | Closed book | 13/03 11.30 - 1.00PM |
| Comprehensive | 40 | 180 min. | Closed book | 08/05 AN |

**\*It will be comprised of surprise tests /computer assignments/presentation.**

**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 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**

