# SEMESTER VI

## CHE-351-MJ-T: PHYSICAL CHEMISTRY III

**Course Type: Major Theory** **Credits: 2**

## D. Course Objectives:

1. To provide foundational knowledge of molecular spectroscopy for understanding molecular structure.
2. To familiarize students with microwave, IR, and Raman spectroscopic techniques and their significance.
3. To introduce concepts of crystal structure and X-ray diffraction methods.
4. To develop insight into kinetics of solid-state reactions and their mechanisms.
5. To build conceptual clarity in spectral interpretation and structural analysis.

## E. Course Outcomes (COs):

| CO No. | Course Outcome Statement (COs)<br>*After learning the course, the students are able to -* |
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| **CO-1** | Recall fundamental concepts of molecular spectroscopy, crystal structure, and solid-state kinetics. |
| **CO-2** | Explain principles of microwave, IR, Raman spectroscopy, and crystallographic methods. |
| **CO-3** | Apply spectroscopic relations and crystallographic equations to solve numerical problems. |
| **CO-4** | Analyze spectral data, crystal parameters, and solid-state reaction kinetics. |
| **CO-5** | Evaluate applications of spectroscopy and X-ray methods in structure determination. |
| **CO-6** | Develop approaches to interpret molecular structure and reaction mechanisms using theoretical concepts. |

## F. Contents:

| **Prerequisites** | |
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| Students should have a basic understanding of atomic structure, chemical bonding, and thermodynamics from undergraduate physical chemistry. Familiarity with basic mathematics (algebra, logarithms) and fundamental concepts of waves and energy. | |
| **Chapter 1: Investigation of Molecular structure** | **14 Hours** |
| **Introduction:** Molar refraction and molecular structure, Dipole moment and molecular | |

structure, electromagnetic spectrum, energy of molecules, Types of molecular spectra

**Microwave Spectroscopy:** Introduction, Classification of molecules on the basis of moment of Inertia, Rotational spectra of rigid diatomic molecules, relative intensities of spectral lines, effect of isotopic substitution on the rotational spectra, Determination of bond length and moment of inertia from rotational spectra, Problems

**Infrared Spectroscopy:** Introduction, Simple Harmonic oscillator, Modes of vibration, force constant, Vibrational spectrum of a diatomic molecule: Vibrational Energy expression, Allowed vibrational energies, zero-point energy, Selection rule, Vibrational energy level diagram with transitions, spectrum depiction, Vibration-rotation Spectra: Born-Oppenheimer approximation, Energy expression for vibrational rotor, Selection rules, Vibrational-rotational energy level diagram with transitions, Nature of vibrational spectra, P, Q and R branches of lines of the IR spectra, Problems.

**Raman Spectroscopy:** Introduction, Classical and Quantum theory of Raman effect, Rayleigh, Stokes and anti-stokes lines, Pure rotational Raman spectra of linear diatomic molecules.

| **Chapter 2: Crystal structure** | **09 Hours** |
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Types of Solids: Isotropy and Anisotropy, Isomorphism and polymorphism, Laws of crystallography: Law of constancy of interfacial angles, Law of rational indices, Law of crystal symmetry, Weiss indices and Miller indices, Crystal Structure: Parameters of the Unit Cells, Cubic Unit Cells: Three Types of Cubic Unit Cells, Calculation of Mass of the Unit Cell, Methods of Crystal structure analysis: The Laue method and Braggs method: Derivation of Bragg's equation, Determination of crystal structure of NaCl by Bragg's method, X ray analysis of NaCl crystal system, Calculation of d and λ for a crystal system, Numerical.

| **Chapter 3: Kinetics of Reactions in the Solid State** | **07 Hours** |
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Some General Considerations, Factors affecting reactions in Solids, Rate Laws for Reactions in Solids , The Parabolic Rate Law, The First-Order Rate Law, The Contracting Sphere Rate Law, The Contracting Area Rate Law, The Prout–Tompkins Equation, Rate Laws Based on Nucleation, Applying Rate Laws, Results of Some Kinetic Studies, The Deaquation-Anation of $[Co(NH_3)_5H_2O]Cl_3$, Two Reacting Solids.

**References:**


1. Fundamentals of Molecular Spectroscopy, C. N. Banwell, E. M. McCash, McGraw-Hill Education, 4th Edition, 1994.
2. Physical Chemistry, Volume 2, N. B. Singh et al., New Age International Publishers,

3. Essentials of Physical Chemistry, B. S. Bahl, G. D. Tuli, S. Chand & Company Ltd.,
4. Principles of Physical Chemistry, B. R. Puri, L. R. Sharma, M. S. Pathania, Vishal Publishing Co., 50th Edition, 2025.
5. Principles of Chemical Kinetics, J. E. House, Academic Press, 2nd Edition, 2007.
6. Physical Chemistry, G. M. Barrow, McGraw-Hill, 6th Edition, 1996.
7. University General Chemistry, C. N. R. Rao, Macmillan, 3rd Edition, 1998.
8. Physical Chemistry, R. A. Alberty, Wiley Eastern Ltd.,
9. The Elements of Physical Chemistry, P. W. Atkins, Oxford University Press, 6th Edition, 2013.
10. Principles of Physical Chemistry, S. H. Maron, C. H. Prutton, Macmillan, 4th Edition, 1965.
11. Quantum Chemistry, D. A. McQuarrie, Viva Books Pvt. Ltd., Student Edition, 2008.
12. Quantum Chemistry, I. N. Levine, Pearson Education, 7th Edition, 2013.
13. Quantum Chemistry, R. K. Prasad, New Age International Publishers, 6th Edition, 2023.
14. Source Book of Atomic Energy, S. Glasstone, Van Nostrand Company, 3rd Edition, 1967.
15. Modern Electrochemistry, J. O'M. Bockris, Plenum Press (Springer), 2nd Edition, 2000.
16. Chemical Applications of Radioisotopes, H. J. M. Brown, Academic Press, Latest Edition.