

**JCL 311 (Aug) (3-0-0)****Molecular Structure and Spectroscopy**

**Instructor: Kanishka Biswas**

Introduction: Electromagnetic spectrum - Different type of molecular energies - Different type of spectroscopy - Probability of transition and selection rules (derivation from perturbation theory) - Einstein absorption coefficient - Absorption and emission spectra - spectral line width

Symmetry and point group: Use in spectroscopy: Symmetry elements and operation - point group - point group of simple chemical compound - character tables and irreducible representation - use in vibrational spectroscopy and determination of hybridization.

Rotational Spectroscopy: Rigid rotor energy level - Selection rule - Intensity of spectral line - Effect of isotopic substitution - Application of spectrum to determine bond strength - Non rigid rotor - polyatomic molecules- Application of rotational spectroscopy.

Infrared and Raman spectroscopy: Part A. Energy of diatomic molecule - Simple harmonic oscillator - Anharmonic oscillator - Diatomic vibrating rotator - Energy level diagram - selection rules of vibration-rotation spectra- Breakdown of the Born-Oppenheimer approximation - Vibrations of polyatomic molecules - influence of rotation on the vibration of poly atomic molecule - Simple examples.

Part B. Classical and quantum theory of Raman effect - Pure rotational Raman spectra - Vibrational Raman spectra - Rule of mutual exclusion - overtone and combination vibration - rotational fine structure - simple structure determination from Raman and infrared spectra.

Electronic spectroscopy: Part A. Electronic structure of atom- Angular and spin moment - coupling of angular momentum - Russel-Saunders coupling - spectroscopic term symbols and selection rule - spectra of alkali metal and hydrogen atom - Franck-Condon principle - electronic-vibrational coupling - d-d transition - charge transfer transition- electronic spectra of molecules-  $\pi$  to  $\pi^*$  transition in organic compound.

Part B. The fates of electronically excited states - Fluorescence & phosphorescence -Dissociation & pre-dissociation - Quantum yield - Quenching (Static & Dynamic) - Resonance energy transfer. Laser spectroscopy: Laser action - Population inversion - Different type lasers - Application (Flash photolysis, Determination of fluorescence lifetime, Femtosecond spectroscopy)  
Principles of magnetic resonance

**Reference Books:**

1. Fundamentals of Molecular Spectroscopy by Banwell & McCash
  2. Chemical Applications of Group Theory by F. A. Cotton
  3. Principles of Fluorescence Spectroscopy by Lakowicz
  4. Modern Spectroscopy by Hollas
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