Course Title: Molecular Structure and Spectroscopy

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1. 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

2. 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.

3. 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 rotator - polyatomic molecules- Application of rotational spectroscopy.

4. 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.

5. Electronic spectroscopy

Part A. Electronic structure of atom- Angular and spin moment - coupling of angular monemtum - Russel-Saunders coupling - spectroscopic term symbols and selection rule - spectra of alkali metal and hydrogen atom - Francck-condon principle - electronic-vibrational coupling - d-d transition - charge transfer transition- electronic spectra of molecules- π to π^* 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

6. Laser spectroscopy

Laser action - Population inversion - Different type lasers - Application (Flash photolysis, Determination of fluorescence life time, Femtosecond spectroscopy)

References:

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