

2000-2001

SSP-S 302

ANDHRA UNIVERSITY
DEPARTMENT OF PHYSICS
II M.Sc. PHYSICS & II M.Sc.(Tech.) ELECTRONICS
III SEMESTER
P302: MOLECULAR SPECTROSCOPY

SYLLABUS

ROTATIONAL SPECTROSCOPY: Rotation of Molecules. Microwave spectrum of diatomic molecule. The effect of isotopic substitution. The non-rigid rotator. The spectrum of non-rigid rotator. Influence of nuclear spin on pure rotational Raman spectra of CO_2 , O_2 , H_2 , N_2 . *Barwell Chapter: 2, Chapter: 4.2.*

VIBRATIONAL SPECTROSCOPY: The vibrating diatomic molecule. Harmonic oscillator energy levels. The anharmonic oscillator. The diatomic vibrating rotator. Infrared vibration – rotation spectra. Raman vibration – rotation spectra. Anharmonicity and its influence on IR and Raman spectrum of CO_2 . *Barwell Chapter: 1, 4.3.* Fundamental vibrations of polyatomic molecules. Symmetry elements and C_{2v} point groups. C_{2v} and C_{3v} Character tables. Direct product representation. Selection rules for IR and Raman spectra. Derivation of reduction formula from orthogonality theorem. Determination of vibrational modes of H_2O and NH_3 molecules. Group vibrational modes of CH_2 in $\text{CCl}_3 - \text{CH}_2 - \text{CCl}_3$ molecule. *Raman. Chapters: 1.2, 4, 6, 8.*

ELECTRONIC SPECTROSCOPY OF DIATOMIC MOLECULES: Classification of electronic state. Molecular orbitals and ground states of single homonuclear diatomic molecules. Selection rules. Vibrational character of electronic transitions. Progressions and sequences. Deslandres table and vibrational constants. Dissociation energy and dissociation products. Hund's coupling cases 'a' and 'b'. Rotational fine structure of electronic vibration transitions. The Fortrat diagram and the band head. Combination relations and evaluation of rotational constants for bands with Q branches. *Barwell. Chapter: 6. Hollas: 6.2.*

ELECTRONIC SPECTROSCOPY OF POLYATOMIC MOLECULES: Walsh M.O. diagram for AH_2 molecules. Molecular orbitals, electronic configuration and states of BeH_2 , BH_2 , CH_2 , NH_2 and H_2O . Non-bonding orbitals and electronic transitions in formaldehyde. *Hollas. Chapter: 6.3.1.*

LASER SPECTROSCOPY:

Laser structure and excitation mechanism of N_2 Laser, CO_2 Laser, Excimer Laser and Free lasers. Single rovibronic level fluorescence. Resonance Raman spectroscopy. CARS and SRS. *Hollas. Chapter: 8.*

TEXT BOOKS:

1. "Fundamentals of Molecular Spectroscopy" - C.N.Barwell.
2. "Group Theory" - K.V.Kamalanathan.
3. "High Resolution Spectroscopy" - J.M.Hollas.
4. "Laser Fundamentals" - W.T.Silfvast.