

II SEMESTER

ESP-S210

P201: Atomic and Molecular Physics

1. ONE ELECTRON ATOMS: Quantum numbers, Term values. Relation between Magnetic dipole moment and angular momentum of an orbiting electron. Stern-Gerlach experiment and electron spin. Spin-orbit interaction and dependence of energy on J value only. Selection rules and fine structure of Hydrogen and ionized Helium. Hyperfine structure of H α line of hydrogen ($l = 1/2$). GKS: 3.3, 3.4, 3.6, 7.2, 7.4. White: 9.2, 9.3, 18.2

2. ONE VALENCE ELECTRON ATOMS: Modified term values (quantum defect) due to lifting of orbital degeneracy by core penetration (penetrating orbits) and core polarization (non-penetrating orbits) by nl electrons. Spin-orbit interaction and fine structure of chief spectral series of sodium. Intensity rules and application to doublets of sodium. Hyperfine structure of $^2P-^2S$ of sodium ($l = 3/2$). White: 5.10, 5.11, 7.3, 8.3. GKS 6.1 to 6.8

3. MANY ELECTRON ATOMS: Indistinguishable particles, bosons, fermions, exchange force, lifting of exchange degeneracy, exchange energy, interaction energy, Auger electrons and spectral series of helium. Pauli's principle. Term values. LS coupling and Hund's rules based on Residual Coulombic interaction. Landé's interval rule. Equivalent and non-equivalent electrons. Terms for ns, np, nd coupling ($ss, s^2, pp, p^2, dd, d^2, sp^2$ configurations). Transition from LS coupling terms from i) np^2 , ii) $np(n+1)s$ of carbon group and iii) $3p4s$,

iv) $3d4s$ of silicon or ionized phosphorus. Selection rules for L, S, J and π transitions for electric dipole radiation. Inter-combination lines. Anomalous Zeeman effect (split terms) in magnesium and calcium. Lasers- stimulated emission, population inversion, cavity resonance frequencies, Einstein coefficients. He-Ne laser, He-He laser. Laser beam characteristics. GKS: 5.6 to 5.11, 11.1, 11.2, 11.4, 11.5, 12.6 to 12.12, 12.14, 12.17, 12.18.

4. ATOMS IN EXTERNAL FIELD: Quantum theory of Zeeman and Paschen-Back effects and application to $^1P-^1S$, $^2P-^2S$, $^3P-^3S$, $^1D-^1P$, $^3D-^3P$, $^5F_1-^3H_1$ transitions. Distinction between Normal Zeeman and Paschen-Back effects. Split pattern of H α line of hydrogen and D_1 and D_2 lines of Sodium. GKS: 9.6, 9.11, 9.13. White: Figs: 10.3, 10.12, 10.14, 13.4, 13.8, 13.9

5. DIATOMIC MOLECULES: Molecular quantum numbers. Bonding and anti-bonding orbitals from LCAO's. Explanation of bond order for N_2 and O_2 and their ions. Removal of bonding and anti-bonding electrons: photoelectronic spectroscopy of O_2 . Rotational spectra and the effect of isotopic substitution. Effect of nuclear spin functions on Raman rotation spectra of H_2 (fermion), D_2 (boson). Vibration-rotation spectra (infrared and Raman). Intensity of vibrational bands of an electronic band system in absorption. (The Franck-Condon principle) BANWELL: 2.1, 2.3, 3.2, 3.3, 4.3, 6.2, 6.1, 3.

6. MOLECULAR VIBRATIONS: Symmetry elements and identification of point groups of AH_3 , A_2H_2 , ABH_3 , AB_2H_2 , $A_2B_2H_2$, AH_3 , ABH_3 type molecules. Properties of irreducible representations and $C_{\infty v}$ character table. Reducible representation and symmetry of fundamental molecular vibrations of H_2O . Structural determination of IR type molecules from the observed and expected fundamental bands of Raman and IR spectra. Group Theory by K.V. RAMAN: 1.1, 1.4, 1.2, 4.4, 6.2, 6.3, 8.5, 8.6. BANWELL: 4.5.

15. 1.5

1. Introduction to Atomic Spectra - H.E. White.

2. Fundamentals of Molecular Spectroscopy - C.N. Banwell.

3. Group Theory and Spectroscopy - Gauri Kumar Sharma.

4. Rotational and Vibrational Spectra - H. Ullmann.