Subject Code : P8PYE2

EC-II: ATOMIC AND MOLECULAR PHYSICS

Unit 1 : Atomic Spectra

Quantum states of electron in atoms – Hydrogen atom spectrum – Electron spin – Stern-Gerlach experiment – Spin-orbit interaction – Two electron systems – LS-JJ coupling schemes – Fine structure – Spectroscopic terms and selection rules – Hyperfine structure - Exchange symmetry of wave functions – Pauli's exclusion principle – Periodic table – Alkali type spectra – Equivalent electrons – Hund's rule

Unit 2: Atoms in External Fields and Quantum Chemistry

Atoms in External Fields : Zeeman and Paschen-Back effect of one and two electron systems -- Selection rules – Stark effect .
Quantum Chemistry of Molecules : Covalent, ionic and van der Waals interactions – Born-Oppenheimer approximation – Heitler-London and molecular orbital theories of H_2 – Bonding and anti-bonding MOs – Huckel's molecular approximation – Application to butadiene and benzene.

Unit 3: Microwave and IR Spectroscopy

Rotational spectra of diatomic molecules – Effect of isotopic substitution – The non-rigid rotor - Rotational spectra of polyatomic molecules – Linear, symmetric top and asymmetric top molecules – Experimental techniques -- Vibrating diatomic molecule – Diatomic vibrating rotator – Linear and symmetric top molecules – Analysis by infrared techniques – Characteristic and group frequencies

Unit 4: Raman Spectroscopy and Electronic Spectroscopy of Molecules

Raman spectroscopy : Raman effect -- Quantum theory of Raman effect – Rotational and vibrational Raman shifts of diatomic molecules – Selection rules.
Electronic spectroscopy of molecules : Electronic spectra of diatomic molecules -- The Franck-Condon principle – Dissociation energy and dissociation products – Rotational fine structure of electronic vibration transitions

Unit 5: Resonance Spectroscopy

NMR: Basic principles – Classical and quantum mechanical description – Bloch equations – Spin-spin and spin-lattice relaxation times – Chemical shift and coupling constant -- Experimental methods – Single coil and double coil methods – High resolution methods.

ESR: Basic principles – ESR spectrometer – nuclear interaction and hyperfine structure – relaxation effects – g-factor – Characteristics – Free radical studies and biological applications.

Books for Study and Reference :

Relevant Chapters in

C. N. Banwell, *Fundamentals of Molecular Spectroscopy* (McGraw Hill, New York, 1981).

B. P. Straughan and S. Walker, *Spectroscopy Vol.I.* (Chapman and Hall, New York, 1976).

R. P. Feynman et al. *The Feynman Lectures on Physics Vol. III.* (Narosa, New Delhi, 1989).

H. S. Mani and G. K. Mehta, *Introduction to Modern Physics* (Affiliated East West, New Delhi, 1991).

A. K. Chandra, *Introductory Quantum Chemistry* (Tata McGraw Hill, New Delhi, 1989).

Pople, Schneiduer and Berstein, *High Resolution NMR* (McGraw Hill, New York).

Manas Chanda, *Atomic Stucture and Chemical Bond* (Tata McGraw Hill, New Delhi, 1991).

Ira N. Levine, *Quantum Chemistry* (Prentice-Hall, New Delhi, 1994).

Arthur Beiser, *Concepts of Modern Physics* (McGraw Hill, New York, 1995).

C.P. Slitcher, *Principles of Magnetic Resonance* (Harper and Row).