CORE - VIII
PHYSICAL CHEMISTRY III [75 Hours]

OBJECTIVES

- To impart knowledge on electrochemistry, photochemistry, quantum chemistry, and spectroscopy
- To study the concepts and principles of electrochemistry, photochemistry, quantum chemistry, and spectroscopy

UNIT – I Electrochemistry – I (15 Hours)

Ions in solutions – Debye – Huckel theory of strong electrolytes – Debye – Huckel – Onsager equation – verification and limitation – Debye – Huckel limiting law and its extension. Electrode – Electrolyte interface - adsorption at electrified interface – electrokinetic phenomena – Tiselius method of separation of proteins – Membrane potential- Lippmann capillary equation – Electrical double layers – Helmholtz Perrin, Gouy- Chapman and Stern models.

UNIT – II Electrochemistry – II (15 Hours)

Polarisation and over voltage – Butler Volmer equation- diffusion current-echange and equilibrium current density-Hydrogen and oxygen evolution reactions. Corrosion and passivation of metals – Pourbaix and Evans diagrams – Prevention of corrosion. Electrochemical energy systems – Primary and secondary batteries – (dry cells, lead acid storage batteries, silver- zinc cell, nickel -cadmium battery) –Fuel cells – Electrodeposition – principles and applications.

UNIT – III Photochemistry (15 Hours)

Absorption and emission of radiation – decay of electronically excited states – radiative and non –radiative processes – Fluorescence and Phosphorescence – Prompt and delayed fluorescence – quenching of fluorescence – static and dynamic quenching; Stern – Volmer equation – Excimers and exciplexes - Kinetics of Photochemical reactions – Photosensitized reactions. Photovoltaic and photogalvanic cells – photoelectrochemical cells – solar cells- solar energy conversion.

UNIT - IV Quantum Chemistry – III (15 Hours)

Theory of chemical bonding – Born – Oppenheimer approximation – LCAO – MO approximation for hydrogen molecule ion and hydrogen molecule – Valence Bond theory of hydrogen molecule – Concept of hybridisation – sp, sp^2 and sp^3 hybridisation – Huckel Molecular orbital (HMO) theory for conjugated π- systems-application to ethylene, butadiene and benzene – Self consistent field approximation – Hartree and Hartree – Fock self consistant field theory .

Unit – V Spectroscopy (15 Hours)

Rotational spectroscopy – Rigid Rotor – Intensity of spectral lines – Effect of isotopic substitution on the rotation spectra . Vibrational spectroscopy – harmonic oscillator –

anharmonic oscillator – Hot bands – selection rules – Overtones and combination frequencies – Fermi Resonance. Raman spectroscopy – Raman effect (quantum theory) - Rotational and Vibrational Raman Spectra – Mutual Exclusion Rule. Electronic spectroscopy – Electronic spectra of diatomic molecules – vibrational coarse structure – Franck – Condon Principle.

Text Books:-

1. S. Glasstone, Introduction to Electro Chemistry, Affiliated East West Press, New Delhi, 1960.
2. D.R. Craw, Principles and applications of Electro chemistry, Chapman and Hall, 1991.
3. J. Robbins, Ions in solution – An Introduction to Electro chemistry, Clarendon Press, Oxford (1972).
4. K.K. Rohatgi Mukherjee, Fundamentals of Photochemistry, Wiley Eastern Ltd., 1978.
5. N.J. Turro, Modern Molecular Photochemistry, Benjamin / Cummings, Menlo park, California (1978).
6. R.K. Prasad, Quantum Chemistry, Wiley Eastern, NewDelhi, 1992.
7. M.W. Hanna, Quantum Mechanics in Chemistry, W.A. Benjamin Inc, London 1965.
8. C.N. Banwell, Fundamentals of Molecular Spectroscopy, Mc Graw Hill, Newyork, 1966.

Reference Books:-

1. J.O.M. Bockris and A.K.N. Reddy, Electrochemistry, Vols, 1 and 2, Plenum, New York. 1977.
2. C.M.A Brett and A.M.O. Brett, Electrochemistry, Principles, Methods and Applications, OUP, Oxford, 1993.
3. R.H. Rieger, Electrochemistry, Chapmann and Hall, New York (1994).
4. P. Delahay, Electrode Kinetics and Structure of Double Layer, Interscience, 1965.
5. J.C. Calvert and J.N. Pitts, Photochemistry, Wiley, London, 1966.
6. R.P. Wayne, Photochemistry, Butterworths, London, 1970.
7. R.P. Cundell and A.Gilbert, Photochemistry, Thomas Nelson, London, 1970
8. C.K. Depuy and O.L. Chapman, Molecular reactions and Photochemistry.
9. A.K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill.
10. D.A. McQuarrie, Quantum Chemistry, University Science Books, Mill Valley, California (1983).
11. P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford, 1983.
12. Raymond chang, Basic Principle of Spectroscopy, McGraw Hill Ltd., New York (1971).
13. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962