COURSE WISE BREAKUP

Fourth Year Seventh Semester

SPECILIZATION PHYSICAL CHEMISTRY

THEORY

COURSE CODE	TITLE	CREDIT HOURS	MARKS
CHEM-471	PAPER-I: PHYSICAL CHEMISTRY	03	100
CHEM-472	PAPER-II: PHYSICAL CHEMISTRY	03	100
CHEM-473	PAPER-III: PHYSICAL CHEMISTRY	03	100

PRACTICALS

COURSE CODE	TITLE	CREDIT HOURS	MARKS
CHEM-471	PAPER-I: PHYSICAL CHEMISTRY	02	50
CHEM-472	PAPER-II: PHYSICAL CHEMISTRY	02	50
CHEM-473	PAPER-III: PHYSICAL CHEMISTRY	02	50

- **Total Credits of the Semester = 15 (theory 09 & practicles 06 credits)**
- **Maximum Marks = 450 (theory 300 & practicles 150 marks)**

4th Year; 7th Semester

PAPER-I

Title of the Course: **PHYSICAL CHEMISTRY** Code: **CHEM-471**

Credit Hours: **03** Marks: **100**

Course Contents:

Statistical Thermodynamics

Description of various systems. Concepts of states, accessible states and distribution. Probability concepts. Maxwell - Boltzmann's statistics for the systems of independent particles. Partition functions. The relationship of partition function to the various thermodynamic functions. Transitional, vibrational and rotational partitional functions and equilibrium constant. Statistical thermodynamics. Applications to equilibrium and chemical kinetics. Bose-Einstein's and Fermi-Dirac's statistics.

Electrochemistry

Electrical Double Layer: Interface. A look into the interface; OHP and IHP. Contact adsorption Gibbs Surface Excess. Potential differences across metal solution interfaces. Outer and surface potential differences. Galvani potential difference. Electrochemical potential difference. Interfacial tension. Electro capillary thermodynamics. Lippmann's
equation. Helmholtz-perrin model, Gouy-Chapmann model. Stern model, and BDM (Bockris-Devanathan-Muller) model. Charge density. Differential capacitance. Shape of capacitance-charge curve. The Capacitance hump.

Electrode Kinetics

Electrochemical devices. Charge transfer processes in the absence and presence of electrical field. The Over potential. Butler-Volmer's equation. The Idea of equilibrium exchange current density. The Symmetry factor. High field and low field approximation. Tafel's equation. Cyclic voltammetry and its applications. Fuel cell, corrosion and its prevention. Electrochemical impedance spectroscopy.

RECOMMENDED BOOKS:

1. Gasser R.P.H. and Richards W.G. "Entropy and Energy Levels" Oxford University Press (1974).

2. Wayatt P.A.H. "The Molecular Basis of Entropy and Chemical Equilibrium" Royal Institute of Chemistry London (1971).
3. Smith E.B. "Basic Chemical Thermodynamics" 4th ed. Oxford University Press (1990).
4. Bockris J.O.M. and Reddy A.K.N. "Modern Electrochemistry" Vol-I and II, 4th ed. Plenum Press, London (2003).
5. Muhammad M. and Amjad M. "Principles of Electrode Kinetics" Rooha Printers, Lahore (2001).
6. Seddon J.M. and Gale J.D. "Thermodynamics and Statistical Mechanics" Royal Soc Chem, UK (2002).
7. Aston J.G. and Fritz J.J. "Thermodynamics and Statistical Thermodynamics" John-Wiley, New York (1987).
8. Albery J., Electrode Kinetics, Clarendon, Oxford (1975).
9. Engel, Thomas and Philip Reid, "Thermodynamics, Statistical Thermodynamics", and Kinetics 1st ed., Benjamin Cummings (2006).
10. Bard A.J. and Faulkner L.R. "Electrochemical Methods" John Wiley & Sons (2001).

4th Year; 7th Semester

PAPER-II

Title of the Course: **PHYSICAL CHEMISTRY** Code: **CHEM-472**

Credit Hours: **03** Marks: **100**

Course Contents:

Polymer Chemistry

Introduction to Polymers. Step-growth Polymerizations. Polymer chain growth. Kinetics of polymer chain growth. Copolymerization. Emulsion Polymerization. Natural and Inorganic Polymers. Physical Aspects of polymers. Molecular Weight of Polymers: Distribution, averages, and methods of determination. Viscosity. Osmometry. Light scattering method. Diffusion. Sedimentation. Optical rotation method. Structure of Polymer Chain: Introduction to chain isomerism, stereochemistry, configurations, and conformations. (not in Hiemenz). Amorphous State of Polymers: In depth examination of polymer conformation, microstructure, and dynamics in the amorphous state. Polymer viscoelasticity: Stress relaxation, mechanical models of polymer

behavior, time-temperature superposition, perhaps rheology. Crystalline State of Polymers: crystallization and kinetics, crystalline structures, experimental methods. Polymer Solutions and Blends:

RECOMMENDED BOOKS:

1. Hiemenz P.C. "Polymer Chemistry: The Basic Concepts" Marcel Dekker (1984).
2. Stevens M.P. "Polymer Chemistry: An Introduction" Oxford University Press (1999).
3. Allcock H.R. and Lampe F.W. "Contemporary Polymer Chemistry" Prentice-Hall
1. (1990).
4. Rudin "The Element of Polymer Science and Engineering" Academic Press (1990).
5. Sperling L.H. "Introduction to Physical Polymer Science" Wiley Interscience (1992).
6. Boyd R.H. and Phillips P.J. "The Science of Polymer Molecules" Cambridge (1993).
7. Malcolm P.S. "Polymer Chemistry" Oxford University Press (2005).
8. Ravue, "Principles of Polymer Chemistry" 2nd ed. Plenum Publishers (2000).

4th Year; 7th Semester

PAPER-III

Title of the Course: **PHYSICAL CHEMISTRY** Code: **CHEM-473**

Credit Hours: **03** Marks: **100**

Course Contents:

Quantum Chemistry

Operators and their properties. Angular momentum. Central field problem. Approximate methods. Perturbation methods and variation principle. Many electron systems. Treatment of simple harmonic oscillator, diatomic rigid rotor. Valence bond and molecular orbital theories. pi-electron calculations.

Molecular Spectroscopy

Interaction of electromagnetic radiation with matter. Symmetry properties of molecules. Microwave and infrared spectroscopy. Rotational, vibrational and rotational-vibrational spectra of diatomic and polyatomic molecules. Electronic spectra of simple molecules. Nuclear magnetic resonance spectroscopy.

RECOMMENDED BOOKS:

1. Micheal D.F. "Elements of Quantum Mechanics" Oxford University Press (2005).
1. Whiffen D. H. "Spectroscopy" Longmans Green and Co. London, (1966).
2. Barrow G. "Molecular Spectroscopy" McGraw Hill (1962).
3. Becker E. D. "High Resolution NMR; Theory & Chemical Application", New York, Academic Press (1980).
1. Graybal J.D. "Molecular Spectroscopy", New York, McGraw-Hill (1988).
2. Griffiths, David J., "Introduction to Quantum Mechanics" 2nd ed., Prentice Hall (2004).
3. Hayward, David O., "Quantum Mechanics for Chemists" 1st ed., John Wiley (2003).
4. House, James E., "Fundamentals of Quantum Mechanics" 2nd ed., Elsevier-Academic Press (2003)

4th Year; 7th Semester

PAPER-I

Title of the Practical: **PHYSICAL CHEMISTRY** Code: **CHEM-471**

Credit Hours: **02** Marks: **50**

1. Determination of partial molar quantities.
2. Determination of free energy changes, standard free energies.
3. Verification of Kohlrausch law.
4. Study of temperature dependence of electrode potentials.
5. Determination of heat of solution, ionic reactions and other experiments from thermochemistry.
6. Determination of molecular weight of a polymer by viscosity method.
7. Precipitation value of electrolytes.
8. Measurement of IR spectra of simple compound and their interpretation.
9. Measurement of cyclic voltammogram of an organic compound and its interpretation.
10. Determination of dipole moment of an organic liquid.
11. Determination of percentage composition of KMnO4-K2Cr2O7 in given solution by spectrometry.
12. Evaluation of pKa value an indicator by spectrometric method.

13. Synthesis of metal oxide nanoparticles and their characterization using IR and XRD techniques.

4th Year; 7th Semester

PAPER-II

Title of the Practical: **PHYSICAL CHEMISTRY** Code: **CHEM-472**

Credit Hours: **02** Marks: **50**

1. Study of multistep reactions.
2. Sugar analysis and inversion studies by polarimetry.
3. Study of isotherms and experiments of surface chemistry.
4. Kinetics of fading of phenolphthalein in alkaline solution.
5. Study of the effect of pH on the rate constant of the reaction between iodide and persulphate ions.
6. Study of the salt effect on the rate constant of the reaction between similar charges of ions.
7. Kinetics of autocatalytic reaction between permanganate and oxalate ions.
8. Determination of energy of activation of the reaction between similar chargers of ions.
9. Kinetics of the reaction between methylorange and peroxodisulphate ions in presence of bromide ions.
10. Stoichiometry of a complex in solution by Job's method.

4th Year; 7th Semester

PAPER-III

Title of the Practical: **PHYSICAL CHEMISTRY** Code: **CHEM-473**

Credit Hours: **02** Marks: **50**

RECOMMENDED BOOKS:

1. Braun R.D. and Walters F. "Application of Chemical Analysis" (1982).
2. David P. "Experiments in Physical Chemistry" 5th ed. (1989).

3. Shoemaker C.W., Nibler G.J.W. and Christian G.D. “Analytical Chemistry” 6th ed. (2004).
4. James A.M. and Prichard F.E. “Practical Physical Chemistry” 3rd ed. Longman (1974).
5. Mowry S. and Ogren P.J., J. Chemical Education, 76(7) (1999).
6. Shoemaker D.P., Garland C.W. and Nibler J.W. “Experiments in Physical Chemistry” McGraw Hills, New York (1989).