ADIKAVI NANNAYA UNIVERSITY
DEPARTMENT OF CHEMISTRY
THIRD SEMESTER
PAPER-I: ADVANCED CHEMICAL KINETICS AND PHYSICAL CHEMISTRY OF POLYMERS
(Effective from the 2016-17 admitted Batch)

UNIT–I

Theories of reaction rates – Potential energy surfaces – Reaction coordinate – theories of unimolecular gas phase reactions – Lindemann hypothesis – Hinshelwood treatment – Reactions in solutions – Kinetic Isotope effect – Linear free energy relationships – Hammett equation – Okamato–Brown Equation – Taft Equation; Chain Reactions H_2–Cl_2,H_2–Br_2 and H_2–O_2 reaction – Explosion limits.

UNIT–II

Complex reactions – Consecutive – Parallel and Opposing reactions – Equilibrium and Steady state technique – Michalies – Menten Models. Flow and relaxation Technique for fast reactions – NMR methods determining exchange rates.

UNIT–III

Characteristics of macro molecules(addition & condensation of polymerization), degree of polymerization. Shapes of macro – molecules, bulk, solution and emulsion polymerization – Co-Polymerization, block and graft copolymers ,Ziegler natta catalysis. The structure and properties of polymers – Crystallinity. Glass-transition temperature ,Rheology and solubility of polymers, processing of polymers –Additives.

UNIT–IV

Interaction of polymers and liquids – Flory – Huggins treatment and its limitation,Fractionation ,Viscosities of polymer solutions, Synthesis and properties of polyesters ,polylamides polyurethanes ,polystyrene and bakelite .Determination of molecular Weights of polymers by osmometry ,light scattering .Ultra centrifuge and Viscometry .

Suggested books :

1. Chemical Kinetics by Laidler.
2. Physical Organic Chemistry by Wiberg.
3. Kinetics and Mechanism by Frost and Pearson.
4. Molecular connectivity in Chemistry and Drug Research L.B.Kier and L.H.Hall Academic press,1976.
5. Chemical Kinetics –The study of Reaction Rates in solution –Kenneth A.CANNORSV– VCH Publishers.
6. An introducer to polymer Chemistry –W.R.Moore.
7. Introduction to polymer Chemistry –R.B.Seymour.
8. Fundamentals of Polymer Science and Engineering –Anil Kumar and S.K.Gupta.

ADIKAVI NANNAYA UNIVERSITY
DEPARTMENT OF CHEMISTRY
THIRD SEMESTER
PAPER II: QUANTUM CHEMISTRY –II AND CHEMICAL APPLICATIONS OF SYMMETRY AND GROUP THEORY
(Effective from the 2016-17 admitted Batch)

UNIT –I:

Wave mechanics of simple systems –Systems with discontinuity in the Potential field –Quantum Mechanical tunneling effect –potential barrier with finite thickness.

Wave mechanics of systems with variable potential energy – Harmonic Oscillator – Hermite polynomials –recursion formula –Energy levels of three dimensional harmonic oscillator – degeneracy of the energy levels.

UNIT –II:

Hydrogen like atoms –Solutions of the wave equation –solution of R(r), ϕ (ϕ) and θ (θ) equations – Shapes of atomic orbitals – Space quantization of electronic orbitals.

Angular momentum – Commutation realations – Commutation with Hamitonian-Spin-Orbit interaction – Vector model of the atom.

UNIT–III:

Representation – reducible and irreducible representations – Orhogonality theorem and its consequences – Constructions of Character table for C_{2v} and C_{3v} point groups – Wave functions as bases for irreducible representations – Direct Product

Hybridization scheme for AB_n type of molecules – AB_3, AB_4, AB_5 and AB_6 under point groups D_{3h} D_{4h}, T_d, C_{4v} and O_h

Ligand field theory: Splitting of d-orbitals under D_{4h}, T_d, C_{4v} and O_h environments.

Construction of molecular orbital correlation diagram (1) for ϭ bonds in octahedral environment and (2) for H_2O molecule.

UNIT-IV:

Symmetry selection rules for I.R. and Raman activity – transition moment integral – appilication of direct product.

Determination of symmetries of total degrees of freedom: Calculation of Chatacter per un-shifted atom for different symmetry operations and evaluation of SF_6.

Determination of symmetries of I.R. and Raman active vibrational modes for different molecules SO_2, NO_2, CCl_4, $POCl_3$, PCl_5 and SF_6.

Accidental degeneracy and Fermi Reasonance.

Recommended Text Books:

1. Chemical Appilications of Group Theory, F.A.Cotton Wiley Eastern Limited, New Delhi.
2. Group Theory and its Appilications to Chemistry, K.V.Ramana, Tata McGraw-Hill Publishing Company Limited New Delhi.
3. Introductory Quantum Chemistry, A.K.Chandra, TATA MCGRAW-HILL Publishing Company Ltd., New Delhi.
4. Quantum Chemistry, Iran Levine, Pearson Education.
5. Theoretical Chemistry, S.Glastone.

ADIKAVI NANNAYA UNIVERSITY
DEPARTMENT OF CHEMISTRY
THIRD SEMESTER
PAPER-III: STATISTICAL THERMODYNAMICS AND SOLUTION EQUILIBRIA OF PROTON LIGAND COMPELXES
(Effective from the 2016-17 admitted Batch)

UNIT-I:

Statistical mechanics : Ensembles (Canonical and micro canonical) –Basic definition distribution and microstates ,thermodynamic probability . The classical distribution law . The Maxwell – Boltzmann distribution law ,method of lagrangian multiplies ,indistinguishable particles, quantum statistics – Bose –Einstein and Fermi Dirac Statistics, Conditions for the applicability of Maxwell – Boltzmann statistics, Bose – Einstein statistics and radiation, extreme gas degeneration, degenerate electron gas.

UNIT-II :

Statistical thermodynamics: Partition function. Thermodynamics functions from partition functions for multiple degree of freedom, theories of heat capcities of solids, stastical evaluation of entropy, comparison of statistical values with third law entropies (thermal entropies).

UNIT-III :

Gran analysis of acid base titrations –Determination of Carbonate content and correction factors for P^H meter dial readings ; Secondary formation function nbarh; Calculation of stability constants of proton ligand complexes –successive approximation method –half nbarh method; Simulation of p^H metric titration data for proton –ligand systems.

UNIT –IV :

Prediction of proton –ligand formation constants using Molecular mechanics/ Quantum Chemical methods; Effect of solvent on stability – Abraham multi layer model –LD model; Components of expert systems – knowledge base, inference engine and user interface.

Suggested Books:

1. M.T.Beck,Complex Equilibria,1991
2. Alcock,solution Equilibria,1992
3. Richard E. Dickerson,Molecular Thermodynamics
4. S.Glasstone, Theoretical Chemistry
5. S.Glasstone,Thermodynamics for Chemists
6. C.Andrews ,Equilibrium Statistical Mechanics
7. Davies, Thermodynamics
8. Yeremin, Thermodynamics
9. J. Rajaram, and T.C. Kuriacose, Thermodynamics for student of chemistry.

ADIKAVI NANNAYA UNIVERSITY
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THIRD SEMESTER

PAPER –IV : INSTRUMENTATION

(Effective from the 2016-17 admitted Batch)

UNIT –I :

Spectrophotometry – deviations from Beer - lamberts law Instrumentation –Errors in Spectrophotometry – photometric titrations composition and stability constants of mononuclear complexes by linear extrapolation methods.Fundamental principles of Fluorescence spectroscopy and basic instrumentation of spectrofluorimeter.

UNIT –II :

Chromatrographic methods - Ion exchange chromatography separation of transition metal ion – solvent extraction - partition coefficient – distribution ratio - classification of solvent extraction systems and evaluation of formation constants and applications Gas liquid Chromatography principal - Instrumentation - retention time - retention volume – Elementrary principles of HPLC and hyphenated instruments.

UNIT –III :

Techniques and instrumentation of IR , Microwave and Raman. Theory and instrumentation Atomic absorption spectroscopy - Atomic emission spectroscopy with ICP source - Elementary principles of laser mass spectrometry.

UNIT – IV :

Polarography - Introduction - types of currents - qualitative and quantitive aspects of polarography – analytical applications to organic and inorganic compounds - Evaluation of stability constants by deford and hume method – amperometric titrations. Principles of thermo gravimetry - Apparatus and working, Differential methods of analysis - principle factors affecting DTA curve. Application of DTA .

Suggested Books:

1. Quantitative Analysis – R.A.Day and A.L.Underwood
2. Quantitative Inorganic Analysis – A . I . Vogel
3. Spectroscopy S.Walker and Straw Volumes I, II and III
4. Instrumental Methods of Chemical Analysis - Kudesla Snwheny (Pragati Prallesan Meerut) 1988.
5. Instrumental Techniques for Analytical Chemistry-Frank settle (Pearson Eddition)2004.