

BRANCH IVA

M.Sc.

ANALYTICAL

CHEMISTRY

FOREWORD

I feel highly privileged in presenting the revised curricula and syllabi of Branch IVA M.Sc. Analytical Chemistry for favour of approval by the Faculty and Academic Council of the University.

As per Mahatma Gandhi University PG Programme Regulations for Credit Semester System 2011(MGU-CSS-PG) it has been decided to introduce the Credit Semester System for all the PG courses which are being offered by the affiliated colleges/institutions of the University with effect from the academic year 2012-2013 admission onwards. The PG Board of Studies in Chemistry was entrusted with the duty of preparing the revised curricula and syllabi for all the five M.Sc. Programmes in Chemistry currently approved by the University and offered in the affiliated colleges.

The BOS prepared draft proposals of revised curricula and syllabi for all the M.Sc. courses in Chemistry in conformity with the broad guidelines issued by the University to suit the Credit Semester System. The draft curricula and syllabi for all the five M.Sc. Programmes were discussed in a very effective manner with active participation of Resource Persons and Teacher Representatives from all the colleges in a three-day workshop. The workshop was a grand success and the BOS could incorporate many of the suggestions while finalizing the proposal of the Restructured Curricula and Syllabi.

The BOS feel that appreciable updating could be done in keeping with the current developments and trends in chemistry education. The task of preparing the Curricula and Syllabi and bringing it out in the present form for all the five M.Sc. courses was not a simple task but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS. I would like to express my sincere thanks to all my fellow members of the BOS for all their whole hearted time-bound help, cooperation and encouragement. It has been a pleasure for me to work with them. I am also thankful to all Resource Persons and Teacher Representatives of the colleges for their active participation and useful suggestions during the three-day workshop.

Prof. (Dr.) P. K. Radhakrishnan
Chairman, PG Board of Studies in Chemistry

PG Board of Studies in Chemistry

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	Code	Course	Hours/ Week	Total Hours	Credit	
Semester 1	AN1C01	Organometallics and Nuclear Chemistry	4	72	4	
	AN1C02	Structural and Molecular Organic Chemistry	4	72	4	
	AN1C03	Quantum chemistry and Group Theory	4	72	4	
	AN1C04	Classical and Statistical Thermodynamics	3	54	3	
	AN2P01	Inorganic Chemistry Practical-1	3	54	Evaluation at the end of 2 nd semester	
	AN2P02	Organic Chemistry Practical-1	3	54		
	AN2P03	Physical Chemistry Practical	4	72		
		Total	25	450	15	
Semester 2	AN2C05	Coordination Chemistry	4	72	4	
	AN2C06	Organic Reaction Mechanisms	4	72	4	
	AN2C07	Chemical Bonding and Computational Chemistry	4	72	4	
	AN2C08	Molecular Spectroscopy	3	54	3	
	AN2P01	Inorganic Chemistry Practical-1	3	54	3	
	AN2P02	Organic Chemistry Practical-1	3	54	3	
	AN2P03	Physical Chemistry Practical	4	72	3	
		Total	25	450	24	
Semester 3	AN3C09	Structural Inorganic Chemistry	4	72	4	
	AN3C10	Organic Syntheses	4	72	4	
	AN3C11	Selected Topics in Physical Chemistry	4	72	4	
	AN3C12	Spectroscopic Methods in Chemistry	3	54	3	
	AN4P04	Inorganic Chemistry Practical-2	3	54	Evaluation at the end of 4 th semester	
	AN4P05	Organic Chemistry Practical-2	3	54		
	AN4P06	Instrumental Analysis Practical	4	72		
		Total	25	450	15	
Semester 4		Elective 1	5	90	4	
		Elective 2	5	90	4	
		Elective 3	5	90	4	
		AN4P04	Inorganic Chemistry Practical-2		54	3
		AN4P05	Organic Chemistry Practical-2	3	54	3
		AN4P06	Instrumental Analysis Practical	4	72	3
		AN4D0	Project			3
		AN4V0	Viva			2
		Total	25	450	26	
Grand Total					80	

SEMESTER 1

AN1C01 ORGANOMETALLICS AND NUCLEAR CHEMISTRY **Credit: 4** **Contact Lecture Hours: 72**

Unit 1: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hours)

- 1.1 Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.
- 1.2 Complexes with cyclic pi donors-metallocenes and cyclic arene complexes-structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.
- 1.3 Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons.

Unit 2: Reactions of Organometallic Compounds (9 Hrs)

- 2.1 Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.
- 2.2 Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.
- 2.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Unit 3: Catalysis by Organometallic Compounds (9 Hrs)

- 3.1 Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.
- 3.2 Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer-Tropsch reaction(synthesis of gasoline).
- 3.3 Hydroformylation of olefins using cobalt or rhodium catalyst.
- 3.4 Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts.
- 3.5 Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $\text{Co}_2(\text{CO})_8$ catalyst in adipic ester synthesis.
- 3.6 Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop"). Palladium catalysed oxidation of ethylene-the Wacker process.

Unit 4: Organometallic Polymers (9 Hrs)

- 4.1 Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Unit 5: Bioinorganic Compounds (18 Hrs)

- 5.1 Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+ , ATP and ADP. Photosynthesis-chlorophyll a, PS I and PS II. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.
- 5.2 Oxygen carriers and oxygen transport proteins-haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems-ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes-CarboxypeptidaseA-structure and functions. Nitrogen Fixation-nitrogenase, vitamin B_{12} and the vitamin B_{12} coenzymes.
- 5.3 Metals in medicine-therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals(Cd, Hg, Cr and Pb).

Unit 6: Nuclear Chemistry (9 Hrs)

- 6.1 Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations. Positron annihilation and autoradiography. Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.
- 6.2 Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.
- 6.3 Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.
- 6.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal. Radiation chemistry of water and aqueous solutions.
- 6.5. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

References

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03. K.F. Purcell, J C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
04. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988.
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08. H.J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1982.
09. S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

AN1C02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY

Credit: 4

Contact Lecture Hours: 72

Unit 1: Basic Concepts in Organic Chemistry (18 Hrs)

- 1.1 Review of basic concepts in organic chemistry: bonding, hybridisation, MO picture, inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.
- 1.2 The formalism of curved arrow mechanisms. Practicing of line diagram drawing.
- 1.3 Concept of aromaticity: delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems - annulenes. NMR as a tool for aromaticity. Anti- and homo-aromatic systems - Fullerenes, Carbon nanotubes and Graphene.
- 1.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. SN1, SNAr, SRN1 and Benzyne mechanisms.

Unit 2: Physical Organic Chemistry and Photochemistry (18 Hrs)

- 2.1 Energy profiles. Kinetic versus thermodynamic control of product formation, Hammond postulate, kinetic isotope effects with examples, Hammett equation, Taft equation. Linear free energy relationships.
- 2.2 Catalysis by acids and bases and nucleophiles with examples from acetal, cyanhydrin and ester formation and hydrolysis reactions-AAC2, AAC1, AAL1, BAC2 and BAL1 mechanisms. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Hard and soft acids and bases - HSAB principle and its applications.
- 2.3 Photoreactions of carbonyl compounds: Norrish reactions of ketones. Paterno-Buchi reaction. Barton, Di- π -methane and photo Fries rearrangements. Photochemistry of nitro and azo groups.

Unit 3: Stereochemistry of Organic Compounds (18 Hrs)

- 3.1 Introduction to molecular symmetry and chirality: examples from common objects to molecules. Axis, plane, center, alternating axis of symmetry.
- 3.2 Center of chirality: molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and Cn, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro, threo nomenclature.
- 3.3 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidenecycloalkanes.

- 3.4 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.
- 3.5 Stereoisomerism: definition based on symmetry and energy criteria, configuration and conformational stereoisomers.
- 3.6 Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

Unit 4: Conformational Analysis

(18 Hrs)

- 4.1 Conformational descriptors - factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems. Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination-Saytzeff and Hofmann eliminations), substitution and oxidation of 2^o alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle.

References

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02. F.A. Carey, R.A. Sundberg, *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, 5th Edn., Springer, 2007.
03. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, 2004.
04. T.H. Lowry, K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 2nd Edn., Harper & Row, 1981.
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09. N.J. Turro, V. Ramamurthy, J.C. Scaiano, *Principles of Molecular Photochemistry: An Introduction*, University Science books, 2009.
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11. K.K.R. Mukherjee, *Fundamentals of Photochemistry*, New Age Pub., 1978.

AN1C03 QUANTUM CHEMISTRY AND GROUP THEORY
Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Postulates of Quantum Mechanics **(9 Hrs)**

- 1.1 State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions.
- 1.2 Operator postulate: operator algebra, linear and nonlinear operators, Laplacian operator, commuting and noncommuting operators, Hermitian operators and their properties, eigen functions and eigen values of an operator.
- 1.3 Eigen value postulate: eigen value equation, eigen functions of commuting operators.
- 1.4 Expectation value postulate.
- 1.5 Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.

Unit 2: Application to Exactly Solvable Model Problems **(18 Hrs)**

- 2.1 Translational motion: free particle in one-dimension, particle in a one-dimensional box with infinite potential walls, particle in a one-dimensional box with finite potential walls-tunneling, particle in a three dimensional box-separation of variables, degeneracy.
- 2.2 Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation(solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.
- 2.3 Rotational motion: co-ordinate systems, cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates-particle on a ring, the phi equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)-polar diagrams of spherical harmonics.
- 2.4 Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x , L_y , L_z and L^2)-commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2 . Ladder operator method for angular momentum. Space quantization.

Unit 3: Quantum Mechanics of Hydrogen-like Atoms (9 Hrs)

- 3.1 Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals-radial functions, radial distribution functions, angular functions and their plots.
- 3.2 The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin-Stern Gerlach experiment. Spin orbitals-construction of spin orbitals from orbitals and spin functions.

Unit 4: Symmetry and Groups (9 Hrs)

- 4.1 Symmetry elements, symmetry operations, point groups and their symbols, sub groups, classes, abelian and cyclic groups, group multiplication tables-classes in a group and similarity transformation.
- 4.2 Symmetry in crystals-32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis. Glide planes. Space groups-determination of space group symbols of triclinic and monoclinic systems.

Unit 5: Theory of Molecular Symmetry (18 Hrs)

- 5.1 Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic orbitals as basis, representation generated by cartesian coordinates positioned on the atoms of a molecule (H₂O and SO₂ as examples).
- 5.2 Reducible and irreducible representations-construction of irreducible representation by standard reduction formula. Statement of Great Orthogonality Theorem (GOT). Properties of irreducible representations. Construction of irreducible representation using GOT-construction of character tables for C_{2v}, C_{2h}, C_{3v} and C_{4v}. Direct product of representations.
- 5.3 Molecular dissymmetry and optical activity.

Unit 6: Application of Group Theory in Spectroscopy (9 Hrs)

- 6.1 Applications in vibrational spectra: transition moment integral, vanishing of integrals, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Determination of the symmetry of normal modes of H₂O, Trans N₂F₂ and NH₃ using Cartesian coordinates and internal coordinates. Complementary character of IR and Raman spectra-determination of the number of active IR and Raman lines.
- 6.2 Application in electronic spectra: selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.

References

01. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.
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17. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010

AN1C04 CLASSICAL AND STATISTICAL THERMODYNAMICS

Credit: 3

Contact Lecture Hours: 54

Unit 1: Classical Thermodynamics (27 Hrs)

- 1.01 Entropy, dependence of entropy on variables of a system (S, T and V; S,T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.
- 1.02 Free energy, Maxwell relations and significance, temperature dependence of free energy - Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.
- 1.03 Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.
- 1.04 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.
- 1.05 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions-free energy, enthalpy, entropy and volume. Determination of excess enthalpy and volume.
- 1.06 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- vant Hoff reaction isochore and isotherm.
- 1.07 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.
- 1.08 Three component systems-graphical representation. Solid-liquid equilibria-ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria-one pair of partially miscible liquids, two pairs of partially miscible liquids, three pairs of partially miscible liquids.
- 1.09 Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, the Onsager reciprocal relations. Thermal osmosis. Thermoelectric phenomena.
- 1.10 Bioenergetics: coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

Unit 2: Statistical Thermodynamics (27 Hrs)

- 2.1 Permutation, probability, apriori and thermodynamic probability, Stirlings approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function-

- translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength.
- 2.2 Calculation of thermodynamic functions and equilibrium constants, statistical interpretation of work and heat, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.
 - 2.3 Need for quantum statistics, Bose-Einstein statistics: Bose-Einstein distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi-Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics.
 - 2.4 Heat capacity of solids- the vibrational properties of solids, Einsteins theory and its limitations, Debye theory and its limitations.

References

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SEMESTER 2

AN2C05 COORDINATION CHEMISTRY

Credits: 4

Contact Lecture Hours: 72

Unit 1: Structural Aspects and Bonding

(18 Hrs)

- 1.1 Classification of complexes based on coordination numbers and possible geometries. Sigma and pi bonding ligands such as CO, NO, CN⁻, R₃P, and Ar₃P. Stability of complexes, thermodynamic aspects of complex formation-Irving William order of stability, chelate effect.
- 1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, *Dq* values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory-M.O energy level diagrams for octahedral and tetrahedral complexes without and with π -bonding, experimental evidences for pi-bonding.

Unit 2: Spectral and Magnetic Properties of Metal Complexes

(18 Hrs)

- 2.1 Electronic Spectra of complexes-Term symbols of *dⁿ* system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for *dⁿ* and *d¹⁰⁻ⁿ* ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.
- 2.2 Interpretation of electronic spectra of complexes-Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of *Dq*, *B* and β (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.
- 2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism-Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism-inter and intramolecular interaction. Anomalous magnetic moments.
- 2.4 Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.

Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes

(18 Hrs)

- 3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, *trans* effect-theory and applications.

- 3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).
- 3.3 Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism.

Unit 4: Stereochemistry of Coordination Compounds (9 Hrs)

- 4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds,
- 4.2 Linkage isomerism-electronic and steric factors affecting linkage isomerism. Symbiosis-hard and soft ligands, Prussian blue and related structures, Macrocycles-crown ethers.

Unit 5: Coordination Chemistry of Lanthanides and Actinides (9 Hrs)

- 5.1 General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents.
- 5.2 General characteristics of actinides-difference between *4f* and *5f* orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

References

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02. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
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11. T. Moeller, *International Review of Science: Inorganic Chemistry, Series I, Vol VII*, Butterworth, 1972.

AN2C06 ORGANIC REACTION MECHANISM

Credit: 4

Contact Lecture Hours: 72

Unit 1: Review of Organic Reaction Mechanisms (9 Hrs)

- 1.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (SN_1 , SN_2 , SN_i , SE_1 , SE_2 , addition-elimination and elimination-addition sequences), elimination (E_1 and E_2) and addition reactions (regioselectivity: Markovnikov's addition-carbocation mechanism, anti-Markovnikov's addition-radical mechanism). Elimination vs substitution.
- 1.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (SN_2 and SN_1) and elimination (E_1 and E_2) reactions.

Unit 2: Chemistry of Carbanions (9 Hrs)

- 2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond ($X = C, O, N$) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates- lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates.
- 2.2 Nucleophilic additions to carbonyls groups. Named reactions under carbanion chemistry-mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.
- 2.3 Ylids: chemistry of phosphorous and sulphur ylids - Wittig and related reactions, Peterson olefination.

Unit 3: Chemistry of Carbocations (9 Hrs)

- 3.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.
- 3.2 C-X bond ($X = C, O, N$) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.
- 3.3 C-C bond formation involving carbocations: oxymercuration, halolactonisation.

Unit 4: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

- 4.1 Structure of carbenes (singlet and triplet), generation of carbenes, addition and insertion reactions.

- 4.2 Rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.
- 4.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.
- 4.4 Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.
- 4.5 Arynes: generation, structure, stability and reactions. Orientation effect-amination of haloarenes.

Unit 5: Radical Reactions (9 Hrs)

- 5.1 Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements-Hydroperoxide: formation, rearrangement and reactions. Autooxidation.
- 5.2 Named reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Unit 6: Chemistry of Carbonyl Compounds (9 Hrs)

- 6.1 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolf-Kishner), addition (addition of cyanide, ammonia, alcohol) reactions, Cannizzaro reaction, addition of Grignard reagent. Structure and reactions of α , β -unsaturated carbonyl compounds involving electrophilic and nucleophilic addition-Michael addition, Mannich reaction, Robinson annulation.

Unit 7: Concerted reactions (18 Hrs)

- 7.1 Classification: electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions. Woodward Hoffmann rules - frontier orbital and orbital symmetry correlation approaches - PMO method.
- 7.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (with stereochemical aspects), dipolar cycloaddition(introductory).
- 7.3 Unimolecular pyrolytic elimination reactions: cheletropic elimination, decomposition of cyclic azo compounds, β -eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.
- 7.4 Problems based on the above topics.

References

- 01. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

02. F.A. Carey, R.A. Sundberg, *Advanced Organic Chemistry, Part B: Reactions and Synthesis*, 5th Edn., Springer, 2007.
03. W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, Cambridge University Press, 2005.
04. J. March, M.B. Smith, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6th Edn., Wiley, 2007.
05. A. Fleming, *Frontier Orbitals and Organic Chemical Reactions*, Wiley, 1976.
06. S. Sankararaman, *Pericyclic Reactions-A Text Book*, Wiley VCH, 2005.
07. R.T. Morrison, R.N. Boyd, S.K. Bhattacharjee, *Organic Chemistry*, 7th Edn., Pearson, 2011.
08. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, 2004.

AN2C07 CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

Credit: 4

Contact Lecture Hours: 72

Unit 1: Approximate Methods in Quantum Mechanics (18 Hrs)

- 1.1 Many-body problem and the need of approximation methods, independent particle model. Variation method, variation theorem with proof, illustration of variation theorem using the trial function $\psi(a-x)$ for particle in a 1D-box and using the trial function e^{-ar} for the hydrogen atom, variation treatment for the ground state of helium atom.
- 1.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.
- 1.3 Hartree Self-Consistent Field method. Spin orbitals for many electron atoms-symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Unit 2: Chemical Bonding (18 Hrs)

- 2.1 Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2 .
- 2.2 Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2 , Be_2 , N_2 , O_2 and F_2 and hetero nuclear diatomic molecules LiH , CO , NO and HF . Bond order. Correlation diagrams, non-crossing rule. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.
- 2.3 Hybridization, quantum mechanical treatment of sp , sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond orders and free valency.

Unit 3: Applications of Group Theory in Chemical Bonding (9 Hrs)

- 3.1 Applications in chemical bonding, construction of hybrid orbitals with BF_3 , CH_4 , PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v} , C_{2h} , C_3 , C_{3v} and D_{3h} point groups. MO diagram for water and ammonia.

Unit 4: Computational Chemistry

(18 Hrs)

(The units 4 and 5 have been designed to expose the students to the field of computational chemistry, which has emerged as a powerful tool in chemistry capable of supplementing and complementing experimental research. The quantities which can be calculated using computational methods, how to prepare the input to get these results and the different methods that are widely used to arrive at the results are introduced here. Detailed mathematical derivations are not expected. Though computer simulations form an important part of computational chemistry, they are not covered in this syllabus.)

- 4.1 Introduction: computational chemistry as a tool and its scope.
- 4.2 Potential energy surface: stationary point, transition state or saddle point, local and global minima.
- 4.3 Molecular mechanics methods: force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions. Mathematical expressions. Parameterisation from experiments or quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.
- 4.4 Ab initio methods: A review of Hartree-Fock method. Basis set approximation. Slater and Gaussian functions. Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.
- 4.5 Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods-variational method, basic principles of Configuration Interaction(CI). Perturbational methods-basic principles of Møller Plesset Perturbation Theory.
- 4.6 General introduction to semiempirical methods: basic principles and terminology.
- 4.7 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).
- 4.8 Model Chemistry-notation, effect on calculation time (cost).
- 4.9 Comparison of molecular mechanics, ab initio, semiempirical and DFT methods.

Unit 5: Computational Chemistry Calculations

(9 Hrs)

- 5.1 Molecular geometry input-cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS / Firefly input file. GAMESS / Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

- 5.2 Identifying a successful GAMESS/ Firefly calculation-locating local minima and saddle points, characterizing transition states, calculation of ionization energies, Koopmans' theorem, electron affinities and atomic charges.
- 5.3 Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.

References

01. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.
02. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
03. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.
04. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.
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07. E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.
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13. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008.
14. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.
15. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.

Softwares

Molecular Mechanics:

1. **Arguslab** available from www.arguslab.com/
2. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

1. **Firefly / PC GAMESS** available from <http://classic.chem.msu.su/gran/gamess/>
2. **WINGAMESS** available from <http://www.msg.ameslab.gov/gamess/>

Graphical User Interface (GUI):

1. **Gabedit** available from <http://gabedit.sourceforge.net/>
2. **wxMacMolPlt** available from <http://www.scl.ameslab.gov/MacMolPlt/>
3. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

AN2C08 MOLECULAR SPECTROSCOPY

Credit: 3

Contact Lecture Hours: 54

Unit 1: Foundations of Spectroscopic Techniques

(27 Hrs)

- 1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width, contributing factors, Doppler broadening, Lamb dip spectrum, Born Oppenheimer approximation, energy dissipation from excited states (radiative and non radiative processes), relaxation time.
- 1.2 Microwave spectroscopy: principal moments of inertia and classification (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{\max} , effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.
- 1.3 Infrared spectroscopy: Morse potential energy diagram, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, disadvantages of dispersive IR, introduction to FT spectroscopy, FTIR.
- 1.4 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.
- 1.5 Electronic spectroscopy: term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model, different types of lasers-solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

Unit 2: Resonance Spectroscopy

(27 Hrs)

- 2.1 NMR spectroscopy : interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.

- 2.2 FTNMR, second order effects on spectra, spin systems (AB, AB₂), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, ¹³C NMR, natural abundance, sensitivity, ¹³C chemical shift and structure correlation, introduction to solid state NMR, magic angle spinning.
- 2.3 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values (g_{||} and g_⊥), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.
- 2.4 An elementary study of NQR spectroscopy.
- 2.5 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes, MB spectra of Fe(II) and Fe(III) cyanides.

References

01. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.
02. G. Aruldas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.
03. P.W. Atkins, Physical Chemistry, ELBS, 1994
04. R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nostrand Reinhold, 1965.
05. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
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07. W. Kemp, NMR in Chemistry-A Multinuclear Introduction, McMillan, 1986.
08. H. Kaur, Spectroscopy, 6th Edn., Pragati Prakashan, 2011.
09. H. Gunther, NMR Spectroscopy, Wiley, 1995.
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11. D.N. Sathyanarayan, Electronic Absorption Spectroscopy and Related Techniques, Universities Press, 2001.
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SEMESTERS 1 AND 2

AN2P01 INORGANIC CHEMISTRY PRACTICAL-1

Credit: 3

Contact Lab Hours: 54+54=108

PART I

Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li. Anions which need elimination not to be given. Minimum eight mixtures to be given.

PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+ , nitrate and phosphate ions.

PART III

Preparation and characterization complexes using IR, NMR and electronic spectra.

- (a) Tris (thiourea)copper(I) complex
- (b) Potassium tris (oxalate) aluminate (III).
- (c) Hexammine cobalt (III) chloride.
- (d) Tetrammine copper (II) sulphate.
- (e) Schiff base complexes of various divalent metal ions.

References

01. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.
02. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
03. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., McMillian, 1968.
04. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.

AN2P02 ORGANIC CHEMISTRY PRACTICAL-1

Credit: 3

Contact Lab Hours: 54+54=108

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

PART II

1. Separation of Organic binary mixtures by chemical/solvent separation methods
2. Separation of organic mixtures by TLC
3. Separation/ purification of organic mixtures by column chromatography

PART III

Drawing the structures of organic molecules and reaction schemes by ChemDraw, Symyx Draw and Chems sketch. Draw the structures and generate the IR and NMR spectra of the substrates and products in the following reactions:

1. Cycloaddition of diene and dienophile (Diels-Alder reaction)
2. Oxidation of primary alcohol to aldehyde and then to acid
3. Benzoin condensation
4. Esterification of simple carboxylic acids
5. Aldol condensation

References

01. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.
02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.
03. F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.
04. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

AN2P03 PHYSICAL CHEMISTRY PRACTICAL

Credit: 3

Contact Lab Hours: 72+72 =144

(One question each from both parts A and B will be asked for the examination)

Part A

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.
2. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by
 - a) Capillary rise method
 - b) Drop number method
 - c) Drop weight method
2. Determination of parachor values.
3. Determination of the composition of two liquids by surface tension measurements

Part B
Computational chemistry experiments

- V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chems sketch.

References

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.
03. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.
04. GAMESS documentation available from:
<http://www.msg.ameslab.gov/gamess/documentation.html>

SEMESTER 3

AN3C09 STRUCTURAL INORGANIC CHEMISTRY

Credits: 4

Contact Lecture Hours: 72

Unit 1: Solid State Chemistry

(18 Hrs)

- 1.1 Structure of solids: Imperfections in solids-point defects, line defects and plane defects. Structure of compounds of AX (Zinc blende, Wurtzite), AX₂ (Rutile, fluorite, antiferite), A_mX₂ (Nickel Arsenide), ABX₃ (Perovskite, Ilmenite). Spinels. Inverse spinel structures.
- 1.2 Solid state reactions-diffusion coefficient, mechanisms, vacancy diffusion, thermal decomposition of solid-Type I reactions, Type II reactions.
- 1.3 Phase transition in solids: classification of phase transitions-first and second order phase transitions, Martensitic transformations, order-disorder transitions and spinodal decomposition. Kinetics of phase transitions, sintering. Growing single crystals-crystal growth from solution, growth from melt and vapor deposition technique.

Unit 2: Electrical, Magnetic and Optical Properties

(18 Hrs)

- 2.1 Kronig-Penney model, Free electron theory, Zone theory and MO theory of solids. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors. Electrons and holes. Mobility of charge carriers. Hall Effect. Pyroelectricity, piezo electricity and ferro electricity. Conductivity of pure metals.
- 2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites.
- 2.3 Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties
- 2.4 Super conductivity-Type I and Type II superconductors, Frolich diagram, Cooper pairs, theory of low temperature super conductors, junctions using superconductors, BCS theory of superconductivity (derivation not required). Super conducting cuprates – YbaCu oxide system, Meisner effect, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes, high temperature superconductors.

Unit 3: Inorganic Chains and Rings

(18 Hrs)

- 3.1 Chains - catenation, heterocatenation. Silicate minerals. Structure of silicates-common silicates, silicates containing discrete anions, silicates containing infinite chains, silicates containing sheets, framework silicates. Silicones. Zeolites-synthesis, structure and applications. Isopoly acids of vanadium, molybdenum and

tungsten. Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications. Phosphate esters in biological systems. Polythiazil-one dimensional conductors.

- 3.2 Rings-topological approach to boron hydrides, Styx numbers. Structure and bonding in borazines, ring silicates and silicones, phosphorous-nitrogen compounds, phosphazenes. Heterocyclic inorganic ring systems-structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems-structure and bonding in sulphur, selenium and phosphorous compounds.

Unit 4: Inorganic Cages and Metal Clusters (9 Hrs)

- 4.1 Cages: synthesis, structure and bonding of cage like structures of phosphorous. Boron cage compounds-Wade Mingos Lauher rules, MNO rule, boranes, carboranes, metallacarboranes.
- 4.2 Metal clusters: dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(\text{Re}_2\text{X}_8)^{2-}$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains.

Unit 5: Chemistry of Materials (9 Hrs)

- 5.1 Glasses, ceramics, composites, nanomaterials-preparative procedures. Sol-gel synthesis, glassy state-glass formers and glass modifiers, ceramic structures-mechanical properties, clay products, refractories- characterizations, properties and applications.

References

01. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
02. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.
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12. C.V. Agarwal, *Chemistry of Engineering Materials*, 9th Edn., B.S. Pub., 2006.

AN3C10 ORGANIC SYNTHESSES

Credit : 4

Contact Lecture Hours: 72

Unit 1: Organic Synthesis via Oxidation and Reduction (18 Hrs)

- 1.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium and DMSO based reagents) (b) alkenes to epoxides (peroxides/per acids based)-Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation (c) alkenes to diols (Manganese and Osmium based)-Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese and lead based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage-hydroboration-oxidation, Wacker oxidation, selenium/chromium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villiger oxidation.
- 1.2 (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson). (b) Metal based reductions- Birch reduction, pinacol formation, acyloin formation (c) Hydride transfer reagents from Group III and Group IV in reductions - LiAlH_4 , DIBAL-H, Red-Al, NaBH_4 and NaCNBH_3 , selectrides, trialkylsilanes and trialkylstannane. Meerwein-Ponndorf-Verley reduction. Baker's yeast.

Unit 2: Modern Synthetic Methods and Reagents (18 Hrs)

- 2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Noyori reaction. Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Suzuki-Miyaura, Negishi-Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Wohl-Ziegler reaction. Reagents such as NBS, DDQ and DCC. Gilman reagent.
- 2.2 Introduction to multicomponent reactions-Click reactions.

Unit 3: Construction of Carbocyclic and Heterocyclic Ring Systems (9 Hrs)

- 3.1 Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered rings-oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Mitsunobu reaction, cation-olefin cyclization and radical-olefin cyclization.
- 3.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Reformatsky reaction. Construction of macrocyclic rings-ring closing metathesis.

- 3.3 Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, imidazole, thiazole and oxazole.

Unit 4: Protecting Group Chemistry (9 Hrs)

- 4.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection. Illustration of protection and deprotection in synthesis.
- 4.2 Protection and deprotection in peptide synthesis: common protecting groups used in peptide synthesis, protecting groups used in solution phase and solid phase peptide synthesis (SPPS).
- 4.3 Functional equivalence and reactivity Umpolung. Role of trimethyl silyl group in organic synthesis.

Unit 5: Retrosynthetic Analysis (9 Hrs)

- 5.1 Basic principles and terminology of retrosynthesis: synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections.
- 5.2 Amine and alkene synthesis: important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Enantioselective synthesis of Corey lactone, longifolene and luciferin. Umpolung equivalent - Peterson olefination, enolate formation, Ireland method.

Unit 6: Biosynthesis and Biomimetic Synthesis (9 Hrs)

- 6.1 Basic principles of the biosynthesis of terpenes, steroids, alkaloids, carbohydrates, proteins and nucleic acids. Biosynthesis of cholesterol, α -terpineol, morphine, glucose and phenyl alanine. Biogenesis of isoprenoids and alkaloids. Biomimetic synthesis of progesterone and sparteine.

References

01. M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.
02. F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.
03. S. Warren, P. Wyatt, Organic Synthesis: The disconnection Approach, 2nd Edn., Wiley, 2008.
04. V.K. Ahluwalia, Oxidation in Organic Synthesis, CRC Press, 2012.
05. I. Ojima, Catalytic Asymmetric Synthesis, 3rd Edn., John Wiley & Sons, 2010.

06. W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, 4th Edn., Cambridge University Press, 2004.
07. J. Clayden, N. Greeves, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
08. R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons, 1994.
09. L. Kuerti, B. Czako, *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier Academic Press, 2005.
10. R.O.C. Norman, J.M. Coxon, *Principles of Organic Synthesis*, 3rd Edn., Chapman and Hall, 1993.
11. V.K. Ahluwalia, L.S. Kumar, S. Kumar, *Chemistry of Natural Products*, CRS Press, 2007.

AN3C11 SELECTED TOPICS IN PHYSICAL CHEMISTRY

Credit: 4

Contact Lecture Hours: 72

Unit 1: Chemical Kinetics and Catalysis

(27 Hrs)

- 1.1 Theories of reaction rates: collision theory-steric factor, potential energy surfaces. Conventional transition state theory-Eyring equation. Comparison of the two theories. Thermodynamic formulation of the two theories. Thermodynamic formulation of the reaction rates. Significance of ΔG^\ddagger , ΔH^\ddagger and ΔS^\ddagger . Volume of activation. Effect of pressure and volume on velocity of gas reactions.
- 1.2 Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions: free radical and chain reactions, steady state treatment, kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Rice-Herzfeld mechanism, branching chains H_2-O_2 , Semonov-Hinshelwood mechanism of explosive reactions, mechanisms of step-growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.
- 1.3 Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.
- 1.4 Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship, kinetic isotope effect.
- 1.5 Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.
- 1.6 Enzyme catalysis and its mechanism, Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.
- 1.7 Mechanisms of heterogeneous catalysis: unimolecular and bimolecular surface reactions, mechanisms of catalyzed reactions like ammonia synthesis, Fischer-Tropsch reactions, hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.

Unit 2: Electrochemistry and Electromotive Force

(9Hrs)

- 2.1 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye-Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye-Huckel limiting equation, deviations from the DHLL.

- 2.2 Polarization - electrolytic polarization, dissolution and decomposition potential, concentration polarization, overvoltage, hydrogen and oxygen overvoltage, mechanism of anodic and cathodic processes (theories of overvoltage), Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants, Tafel equation and its significance.

Unit 3: Crystallography

(9 Hrs)

- 1.1 Methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.
- 1.2 Structure factor: atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.
- 1.3 Liquid crystals: mesomorphic state, types, examples and applications of liquid crystals. Theories of liquid crystals. Photoconductivity of liquid crystals.

Unit 4: Surface Chemistry

(9Hrs)

- 2.1 Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, general properties of emulsions, foam structure, aerosols, surface films, surface pressure and surface potential and their measurements and interpretation. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.
- 2.2 Adsorption: Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.
- 2.3 Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

Unit 5: Photochemistry

(18 Hrs)

- 3.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere.
- 3.2 Principle of utilization of solar energy, solar cells and their working.
- 3.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type,

effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

References

01. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
02. K.J. Laidler, Chemical kinetics, 3rd Edn., Harper&Row, 1987.
03. C. Kalidas , Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.
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05. P.W. Atkins, Physical Chemistry, ELBS, 1994.
06. D.A. McQuarrie, J.D. Simon, Physical chemistry: A Molecular Approach, University Science Books, 1997
07. S. Glasstone, Introduction to Electrochemistry, Biblio Bazar, 2011.
08. D. R. Crow, Principles and Applications of Electrochemistry, 4th Edn., S. Thomes, 1994.
09. B.K. Sharma, Electrochemistry, Krisna Prakashan, 1985.
10. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
11. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.
12. A.R. West, Basic Solid State Chemistry, John Wiley & Sons, 1999.
13. A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, 6th Edn., John Wiley & sons, 1997.
14. K.K. Rohatgi-Mukherjee, Fundamentals of photochemistry, 2nd Edn., New Age International, 1986.
15. G. Aruldas, Molecular structure and Spectroscopy, PHI Learning, 2007.

AN3C12 SPECTROSCOPIC METHODS IN CHEMISTRY

Credit : 3

Contact Lecture Hours: 54

Unit 1: Ultraviolet-Visible and Chiroptical Spectroscopy (9 Hrs)

- 1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.
- 1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions. Chiroptical properties-ORD, CD, octant rule, axial haloketone rule, Cotton effect.
- 1.3 Problems based on the above topics.

Unit 2: Infrared Spectroscopy (9 Hrs)

- 2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituents, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.
- 2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.
- 2.3 Problems on spectral interpretation with examples.

Unit 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

- 3.1 Magnetic nuclei with special reference to ^1H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^1H and ^{13}C NMR scales.
- 3.2 Spin-spin splitting: AX, AX₂, AX₃, A₂X₃, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling-epi, peri and bay effects. NOE. NOE and cross polarization.
- 3.3 Simplification non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling.
- 3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY
- 3.5 Polarization transfer. Selective Population Inversion. DEPT, INEPT and RINEPT. Sensitivity enhancement and spectral editing, MRI.
- 3.6 Problems on spectral interpretation with examples.

Unit 4: Mass Spectrometry**(9 Hrs)**

- 4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, PD, Field Desorption Electrospray Ionization. Fragmentation patterns-nitrogen and ring rules. McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.
- 4.2 Problems on spectral interpretation with examples.

Unit 5: Structural Elucidation Using Spectroscopic Techniques**(9 Hrs)**

- 5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^1H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).
- 5.2 Interpretation of the given UV-Vis, IR and NMR spectra.

References

01. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole, 2000.
02. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.
03. L.D. Field, S. Sternhell, J.R. Kalman, Organic Structures from Spectra, 4th Edn., John Wiley & sons, 2007.
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05. D.F. Taber, Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, Oxford University Press, 2007.
06. H. Gunther, NMR Spectroscopy, 2nd Edn., Wiley, 1995.
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08. D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6th Edn., McGraw-Hill, 2008.
09. W. Kemp, Organic Spectroscopy, 2nd Edn., Macmillan, 1987.
10. F. Bernath, Spectra of Atoms and Molecules, 2nd Edn., Oxford University Press, 2005.
11. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.
12. Online spectral databases including RIO-DB.

SEMESTER 4

ELECTIVE COURSES

(Any 3 courses to be opted from the following courses)

AN4E01 ANALYTICAL PROCEDURES

Credit: 4

Contact Lecture Hours: 90

Unit 1: Risks and Hazards of Chemicals and Procedures (9 Hrs)

- 1.1 Hazards of handling ordinary, corrosive and poisonous chemicals.
- 1.2 Fire hazards. Handling Carcinogens. Toxicology of Cd, Pb, Hg, As, Se, Pu, oxides of nitrogen and sulphur, benzene, halogenated hydrocarbons, aromatic amino compounds, benzopyrene and related compounds. Treatment of hazardous waste and their disposal.
- 1.3 Radiochemical wastes-technique of safe disposal of radiochemical wastes.

Unit 2: Errors in Chemical Analysis (18 Hrs)

- 2.1 Systematic and random errors. Distribution of experimental results. Statistical treatment- standard deviation, variance, confidence limits, application of statistics to data treatment and evaluation, student-t and f tests, detection of gross errors, rejection of a result-Q test, estimation of detection limits.
- 2.2 Least square method, correlation coefficient and its determination.
- 2.3 Hypothesis testing using statistical analysis.
- 2.4 Using spread sheets for plotting calibration curves. Quality assurance and control charts.

Unit 3: Conventional Analytical Procedures (27 Hrs)

- 3.1 Gravimetry: solubility product and properties of precipitates-nucleation, growth and aging, co-precipitation and post precipitation, drying and ignition.
Inorganic precipitating agents: NH_3 , H_2S , H_2SO_4 , H_2PtCl_6 , $\text{H}_2\text{C}_2\text{O}_2$, $(\text{NH}_4)_2\text{MoO}_4$ and NH_4SCN .
Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-l-naphthol, BPHA, dithiocarbamates, sodium tetraphenyl boron, nioxime and nitron.
- 3.2 Acid-Base, redox and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions. Titrations in non-aqueous media. Different solvents and their selection for a titration. Indicators for non-aqueous titrations. Applications.

Variation of potential during a redox titration, formal potential during a redox titration, requirements and detection of the end point in redox titrations, typical titrants like KMnO_4 , $\text{K}_2\text{Cr}_2\text{O}_7$, Ce(IV) , Mn(III) , I , Cl^- , $\text{S}_2\text{O}_3^{2-}$.

Precipitation reactions-titration curves, determination of end points (colored precipitates, colored soluble compounds), adsorption indicators, turbidity methods. Typical examples.

- 3.3 Complexometric titrations: titration curves, types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators, theory of visual use of metal indicators, typical examples of titrants - murexide, eriochrome black T, Patton and Reeder's indicators, calcon, calmagite, calcichrome bromopyrogallol red, xylenol orange, thymolphthalein complexone, zincon, variamine blue.

Unit 4: Sampling

(18 hrs)

- 4.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non-essential water, absorbed and occluded water, determination of water (direct and indirect methods).
- 4.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl , H_2SO_4 , HNO_3 , HClO_4 , HF , microwave decompositions, combustion methods, use of fluxes like Na_2CO_3 , Na_2O_2 , KNO_3 , NaOH , $\text{K}_2\text{S}_2\text{O}_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

Unit 5: Applied Analysis

(9 hrs)

- 5.1 Analytical procedures involved in environmental monitoring. Water quality-BOD, COD, DO, nitrite, nitrate, iron, fluoride.
- 5.2 Soil- moisture, salinity, colloids, cation and anion exchange capacity.
- 5.3 Air pollution monitoring sampling, collection of air pollutants- SO_2 , NO_2 , NH_3 , O_3 and SPM.
- 5.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis.

Unit 6: Analysis of Nano Materials

(9 hrs)

- 6.1 Introduction to nanochemistry: synthesis, characterization and applications of nano materials.

References

01. J.M. Mermet, M. Otto, R. Kellner, Analytical chemistry, Wiley-VCH, 2004.
02. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
03. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
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12. T. Pradeep, Nano: the Essentials, Tata McGraw Hill, 2007.
13. K.W. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, 2nd Edn., Wiley, 2009.
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15. W. Horwitz (Editor), Official Method of Analysis of AOAC International, 18th Edn., AOAC, 2010
16. British Pharmacopeia, TSO, 2012.

AN4E02 INSTRUMENTAL METHODS OF ANALYSIS

Credit: 4

Contact Lecture Hours: 90

Unit 1: Introduction to Instrumental Methods

(18 Hrs)

- 1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods - precision, sensitivity, selectivity, and detection limits.
- 1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio—hardware and software methods.
- 1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

Unit 2: Molecular Spectral Measurements

(18 Hrs)

- 2.1 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments-sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.
- 2.2 Molecular fluorescence and fluorometers: photoluminescence and concentration-electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Introduction to photoacoustic spectroscopy.
- 2.3 IR spectrometry: instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR instruments. MidIR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.
- 2.4 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman spectroscopy in inorganic, organic, biological and quantitative analysis.
- 2.5 NMR spectrometry-magnets, shim coils, sample spinning, sample probes (^1H , ^{13}C , ^{31}P). Principle of MRI.

Unit 3: Atomic Spectral Measurements

(27 Hrs)

- 3.1 Atomic emission and atomic absorption phenomena: comparison of relative merits and drawbacks. Instrumentation details of AAS. Atomisation methods-flame, electrothermal and plasma techniques, glow discharge and laser ablation, sources: HCl, EDL-TGL, wavelength choice detectors, use in qualitative and quantitative analysis, interferences in measurements-chemical, spectral, and instrumental background correction techniques. Atomic emission spectroscopy-flame, arc, spark, plasma emissions (ICP and DCP), details of wave selection-

detection systems, applications.

- 3.2 Atomic X-ray spectrometry: emission of X-ray, absorption process, fluorescence, instrumentation: X-ray tube, radio isotope filters and monochromators, X-ray detectors and transducers, photon counting, gas filled transducers, Geiger tube, counters, signal processors. Application in quantitative and qualitative analysis. Diffraction methods.

Unit 4: Mass Spectrometry (9 Hrs)

- 4.1 Ion sources - EI, CI, FI, MALDI, Electrospray and FAB, Instrumental components - mass analyzers, magnetic sector, double focussing, quadrupole, TOF, Ion trap, FT instruments. Applications in identification of pure compounds, molecular formula, compound identification from comparison spectra, analysis of mixtures by hyphenated methods, quantitative applications. Application of MS with GC, HPLC.

Unit 5: Surface Study Techniques - Instrumentation and Applications (9 Hrs)

- 5.1 Spectroscopic methods: ISS, SIMS, ESCA, AES, AAS.
5.2 Microscopic methods: SEM, STM, AFM.

Unit 6: Research Methodology of Chemistry (9 Hrs)

- 6.1 The search of knowledge, purpose of research, scientific methods, role of theory, characteristics of research.
6.2 Types of research: fundamental research, applied research, historical and experimental research.
6.3 Chemical literature: primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: ScienceDirect, SciFinder. Chemical Abstract.
6.4 Scientific writing: research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.
6.5 Important scientific and chemistry journals. Impact factor.

References

01. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
02. H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis, 5th Edn., Van Nostrand, 1974.

03. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn&Bacon, 1986.
04. W.W. Wendladt, Thermal Methods of Analysis, Interscience, 1964.
05. T. Hatakeyama, F.X. Quinn , Thermal Analysis, John Wiley&Sons, 1999.
06. H.F. Ebel, C. Bliefert and W.E. Russey, The Art of Scientific Writing, Wiley-VCH, 2004.
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08. R. Wiesendanger, Scanning Probe Microscopy and Spectroscopy, Cambridge University Press, 1994.
09. R.L. Dominoswki, Research Methods, Prentice Hall, 1981.
10. W.Best, J.V. Kahn, Research in Education, 10th Edn., Pearson/Allyn&Bacon, 2006.
11. B.E. Cain, The Basis of Technical Communication, ACS, 1988.

AN4E03 MODERN ANALYTICAL TECHNIQUES AND GREEN CHEMISTRY

Credit: 4

Contact Lecture Hours: 90

Unit 1: Electro Analytical Methods (27 Hrs)

- 1.1 Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. Chemfets-importance of specially designed amplifier systems for ion selective electrode systems. Potentiometric titrations-types and applications.
- 1.2 Polarography and voltametric techniques: micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography.
- 1.3 Amperometry: biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry-different types of electrodes and improvements of lower detection limits. Voltammetric sensors. Organic polarography.

Unit 2: Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)

- 2.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection methods, applications. Capillary gel electrophoresis. Capillary isotachopheresis. Isoelectric focusing.
- 2.2 Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography.

Unit 3: Thermal and Radiochemical Methods (9 Hrs)

- 3.1 Thermogravimetry(TG), Differential Thermal Analysis(DTA) and Differential Scanning Calorimetry(DSC) and their instrumentation. Thermometric Titrations.
- 3.2 Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods.

Unit 4: Chromatography**(27 Hrs)**

- 4.1 Classification, migration rates of solutes, important relationships Gas chromatography, GSC and GLC Instrumentation-preparation of column and column materials, temperature, effects, different types of detectors, capillary columns-bonded and cross linked phases, chiral stationary phases, selectivity factors, applications.
- 4.2 Liquid Chromatography: column efficiency, band broadening and the factors affecting it, particle size. HPLC-its instrumentation pumps, sample injection, columns, solvent selection and detectors. Partition chromatography-bonded phase.
- 4.3 Ion exchange chromatography-ion exchange equilibria, packings, detectors, applications.
- 4.4 Size Exclusion Chromatography- columns and limits of permeation and exclusion, applications.
- 4.5 Planar Chromatography-methodology, materials for stationary phases, applications. Paper chromatography.
- 4.6 Supercritical fluid chromatography: properties of supercritical fluids, operating variables in instrumentation, stationary and mobile phases, comparison with the techniques, applications, supercritical fluid extraction, advantages, applications.

Unit 5: Process Instrumentation**(9 Hrs)**

- 5.1 Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N analysers.

Unit 6: Green Chemistry**(9 Hrs)**

- 6.1 Principles of green chemistry, atom economy, principles of green organic synthesis, green alternatives of organic synthesis-coenzyme catalysed reactions, green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalysed synthesis, condensation reactions. Green photochemical reactions.
- 6.2 Green Solvents: ionic liquids, supercritical CO₂, fluoros chemistry.
- 6.3 General principles of microwave assisted organic synthesis.

References

01. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
02. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
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04. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
05. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis , 5th Edn., John Wiley & sons, 1989.
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11. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.
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14. W. Horwitz (Editor), Official Method of Analysis of AOAC International, 18th Edn., AOAC, 2010
15. British Pharmacopeia, TSO, 2012.

AN4E04 APPLIED ANALYSIS AND AQUATIC RESOURCES
Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Environmental Analysis **(18 Hrs)**

- 1.1 Water Analysis: sampling and preservation of water. Determination of pH, EC, TDS, DO, CO₂, alkalinity (carbonate, bicarbonate, hydroxide and total), salinity, chloride, fluoride, sulphate, H₂S, calcium, magnesium, sodium, potassium, iron (total ferrous and ferric), ammonia, nitrite, nitrate, phosphorous (total inorganic and organic), BOD, COD, phenols, surfactants, pesticides, E-Coli and total bacteria. Quality of water, standards of raw and treated water, objectives of waste water treatment. A brief idea of sedimentation, coagulation and flocculation, filtration, disinfection of water. Activated sludge process, trickling filters, sludge treatment and disposal. Softening of water, corrosion and its control. Removal of toxic compounds, refractory organics, and dissolved inorganic substances. Reverse osmosis.
- 1.2 Air Analysis: atmospheric pollution, classification of air pollutants, sources of air pollution and methods of control, sampling of aerosols, sampling of gaseous pollutants, analysis of SO_x, NO_x, CO-CO₂, hydrocarbons, particulates, effects of air pollutants on animals, ozone layer, chlorofluorocarbons, acid rain, greenhouse effect.
- 1.3 Soil/Sediment analysis: a brief idea of chemistry of soil. Trace element analysis in soil - B, Cd, Cu, Fe, Mn, Mo, Zn, Pb. Pesticides and pollution, classification and degradation of pesticides, methods of pesticides analysis. Sampling of soil, aquatic sediments, pH, electrical conductivity, redox potential, alkalinity, inorganic and organic contents.
- 1.4 Waste Management: waste management approaches - waste reduction, recycling, disposal. Management of hazardous wastes, household waste, municipal and industrial wastes-collection, transportation and disposal options.

Unit 2: Biochemical and Clinical Analysis **(9 hrs)**

- 2.1 Cell fractionation techniques-cell lysine: differential and density gradient centrifugation, salting in, salting out, dialysis, ultracentrifugation, electrophoretic techniques-polyacrilamide gel electrophoresis, SDS-PAGE, agrose gel electrophoresis.
- 2.2 Liver function tests, gastric function tests, kidney function tests and glucose tolerance tests. Screening of metabolic diseases.

Unit 3: Forensic Analysis**(18 Hrs)**

- 3.1 Forensics-basic principles and significance, history and development. Crime-definition, crime scene, protection and recording of crime scene, physical clues, processing of crime scene.
- 3.2 Finger prints: classification, conventional methods of development of finger prints-fluorescent and chemical methods. Application of laser and other radiations to development of latent finger print. Foot prints, tyre marks, bite marks and lip prints.
- 3.3 Questioned Document Examination (QDE): forged documents and currency notes. UV counterfeit note detector.
- 3.4 Forensic Ballistics-fire arms, classification and characteristics, analysis of gunshot residues, mechanism of GSR, instrumental methods of GSR analysis.
- 3.5 Explosives: introduction, types, preliminary screening at crime scene, presumptive test (colour and spot test), micro chemical methods of analysis.
- 3.6 Fire Extinguishers and its chemistry, analysis of Arson exhibits by instrumental methods, management of flammable and combustible materials.
- 3.7 Counterfeit coins-AAS analysis, purity of Gold-analysis by XRF / EDXRF.
- 3.8 Forensic Toxicology: classification of poisons, estimation of poisons and drugs with chromatographic, neutron activation analysis and spectrophotometric methods.

Unit4: Food Chemistry and Food Analysis**(36 Hrs)**

- 4.1 Food chemistry: definition and importance. Water in food, water activity and shelf life of food. Carbohydrates-chemical reactions, functional properties of sugars and polysaccharides in foods. Lipids: classification and use of lipids in foods, physical and chemical properties, effects of processing on functional properties and nutritive value. Protein and amino acids-physical and chemical properties, distribution, amount and functions of proteins in foods, functional properties, effect of processing-loss of vitamins and minerals due to processing. Pigments in food, food flavours, browning reaction in foods. Enzymes in foods and food industry, bio-deterioration of foods, food contaminants, additives and toxicants.
- 4.2 Principles of food processing: scope and importance of food processing. Principles and methods of food preservation-freezing, heating, dehydration, canning, addition of additives, fermentation, irradiation, extrusion cooking, hydrostatic pressure cooking, dielectric heating, microwave processing, aseptic processing, hurdle technology, membrane technology. Storage of food-modified atmosphere packaging, refrigeration, freezing and drying of food, minimal processing, radiation processing.
- 4.3 Food microbiology: history of microbiology of food, microbial growth pattern, physical and chemical factors influencing destruction of micro-organisms. Types of micro-organisms normally associated with food-mold, yeast and bacteria.

Micro-organisms in natural food products and their control. Contaminants of food-stuffs, vegetables, cereals, pulses, oil seeds, milk and meat during handling and processing. Biochemical changes caused by micro-organisms, deterioration of various types of food product. Food poisoning and microbial toxins, microbial food fermentation, standards for different foods. Food borne intoxicants and mycotoxins.

- 4.4 Advanced techniques of food analysis: role of analysis and various methods of sampling and analysis of results. Principles and application of flame photometry, atomic absorption, X-ray analysis, electrophoresis, mass spectroscopy, NMR, chromatography, refractometry, rheology, measurements, enzymatic methods, DSC, SEM, rapid methods of microbial analysis, immunoassays, ESR.

Unit 5: Aquatic Resources

(9Hrs)

- 5.1 Aquatic resources: renewable and non-renewable resources-estimation, primary productivity, regional variations. Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion-exchange and hydrate formation methods. Relative advantages and limitations of the methods. Scale formation and its prevention in distillation process.
- 5.2 Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of halides, magnesium, potassium, gold.

References

01. B.B. Nanda, R.K. Tewari, Forensic Science in India: A Vision for the Twenty-first Century, Select Pub., 2001.
02. A.S. Osborn, Questioned Documents, 2nd Edn., Rawman & Littlefield Pub., 1974.
03. M.K. Mehta, Identification of Thumb Impression and Cross Examination of Finger Print Experts, N.M. Tripathi Pub., 1963.
04. M. Johari, Identification of Firearms, Ammunition and Firearm Injuries, BPR&D, 1980.
05. J.D. DeHaan, Kirk's Fire Investigation, 5th Edn., Prentice Hall, 2002.
06. M. Prakash, C.K. Arora, Methods in Toxicology, Anmol Pub., 1998.
07. P. Fellows, Food Processing Technology: Principles and Practice, CRC Press, 2000.
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09. P.M. Davidson, J.N. Sofos, A.L. Branen, Antimicrobials in Foods, 3rd Edn., CRC Press, 2005.
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11. G.G. Birch, M. Spencer, A.G. Cameron, Food Science, 3rd Edn., Pergamon Press, 1986.
12. J. A. Nathanson, Basic Environmental Technology, 5th Edn., Pearson Prentice Hall, 2007.
13. C.W. Jefford, K.L. Rinehart, L.S. Shield, Pharmaceuticals and the Sea, Technomic Pub., 1988.

14. E.D. Howe, Fundamentals of Water Desalination, M.Dekker, 1974.
15. H-G. Heitmann, Saline Water Processing, VCH, 1990.
16. G. M. Masters, W. Ela, Introduction to Environmental Engineering and Science, 3rd Edn., Prentice Hall, 1998.
17. C.S. Rao, Environmental Pollution Control Engineering, New Age International, 1995.
18. Metcalf, Eddy, Waste Water Engineering, Tata McGraw Hill, 2003.
19. H. Wright, A Hand book of Soil Analysis, Logos Press, 1994.
20. T.G. Spiro, K. Purvis-Roberts, W.M. Stigliani, Chemistry of the Environment, University Science Books, 2011.
21. N.P. Cheremisinoff, Biotechnology for Waste and Wastewater Treatment, William Andrew, 1996.

SEMESTERS 3 AND 4

AN4P04 INORGANIC CHEMISTRY PRACTICAL-2

Credit: 3

Contact Lab Hours: 54+54 =108

PART I

Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods.

PART II

Analysis of one of the alloys of brass, bronze and solder. Analysis of one of the ores from hematite, chromite, dolomite, monazite, illmenite.

References

01. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
02. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., Mc Millian, 1968.
03. G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.
04. N.H. Furman, Standard Methods of Chemical Analysis: Vol. 1, Van Nostrand, 1966.
05. F.J. Welcher, Standard Methods of Chemical Analysis: Volume 2, R.E. Kreiger Pub., 2006

AN4P05 ORGANIC CHEMISTRY PRACTICAL-2

Credit: 3

Contact Lab Hours: 54+54=108

PART I

- 1.1 Standard quantitative analysis of milk, butter, oils, fats, starch, glucose, vitamins and medicinal preparations.
- 1.2 Estimation of the number of acetyl, methoxyl, phenolic, amino, nitro, carboxyl, ester, ether and carbonyl groups in organic compounds.

PART II

- 2.1 Designing of multistep Synthetic Sequences with mechanism and Prediction of FTIR, UV-Visible, ^1H and ^{13}C NMR spectra of the substrates and products at each stage
- 2.2 Prediction of the structure of unknown simple organic compound based on the given FTIR, UV-Visible, ^1H and ^{13}C NMR spectra. (About 50 compounds have to be practiced).

PART III

- 3.1 Microwave assisted Organic Synthesis.
- 3.2 Preparation Involving Multistep Synthetic Sequences by the Green Alternatives of Chemical Methods.

Questions will have equal weight age for part I and II. Part III non evaluative.

References

01. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.
02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.
03. F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.
04. J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

AN4P06 INSTRUMENTAL ANALYSIS PRACTICAL

Credit: 3

Contact Lab Hours: 72+72=144

Section A

I. Nephelometry

1. Determination of sulphate.
2. Determination of halides.

II. Chemical Kinetics

1. Determination of the rate constant of the hydrolysis of ester by sodium hydroxide.
2. Determination of Arrhenius parameters.
3. Kinetics of reaction between $K_2S_2O_8$ and KI
4. Influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI
5. Iodination of acetone in acid medium.

III. Polarimetry

1. Kinetics of the inversion of sucrose in presence of HCl.
2. Determination of the concentration of a sugar solution
3. Determination of the concentration of HCl.
4. Determination of the relative strength of acids.

IV. Refractometry

1. Identification of pure organic liquids and oils.
2. Determination of molar refractions of pure liquids.
3. Determination of concentration of solutions (KCl-water, glycerol-water)
4. Determination of molar refraction of solids.
5. Study of complex formation between potassium iodide and mercuric iodide system.

Section B

V. Polarography and related experiments.

1. Determination of half wave potential.
2. Determination of Cd by (a) standard series (b) Standard addition (c) pilot ion method.
3. Determination of organic compounds.

VI. Conductivity measurements

1. Verification of Onsager equation.
2. Determination of the degree of ionization of weak electrolytes.
3. Determination of pK_a values of organic acids.
4. Determination of solubility of sparingly soluble salts.
5. Titration of a mixture of acids against a strong base.
6. Titration of a dibasic acid against a strong base.

VII. Potentiometry

1. Determination of single electrode potentials (Cu and Zn)
2. Application of Henderson equation.
3. Titration of a mixture of acids against a strong base.
4. Determination of the concentration of a mixture of Cl⁻, and I⁻ ions.

VIII. Electrogravimetric estimation of Cu, Ni, and Pb

IX. Flame Photometry

Determination of Na⁺, Li⁺, K⁺ and Ca²⁺.

The examination will be for 6 hours with one experiment each from section A and section B and will have equal weight.

References

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
02. B. Viswanathan, Practical Physical Chemistry, Viva Pub., 2005.
03. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.