

Course structure for M. Sc.

(Chemistry)



(Effective from July 2012)

Department of Chemistry
Faculty of Science
Banaras Hindu University
Varanasi-221005

(To be implemented from Session 2012-13)

Semester -I

1 Credit = 1 hour/week

Course Code	Title	Credits
CHM101	Analytical Chemistry I	3
CHM102	Inorganic Chemistry I	3
CHM103	Organic Chemistry I	3
CHM104	Physical Chemistry I	3
CHM105	Inorganic Chemistry Practical	2
CHM106	Organic Chemistry Practical	2
CHM107	Physical Chemistry Practical	2
	Total:	18
<u>Semester-II</u>		
CHM201	Analytical Chemistry II	3
CHM202	Inorganic Chemistry II	3
CHM203	Organic Chemistry II	3
CHM204	Physical Chemistry II	3
CHM205	Chemical Binding	3
CHM206	Inorganic Chemistry Practical	2
CHM207	Organic Chemistry Practical	2
CHM208	Physical Chemistry Practical	2
CHM209M	Polymer Chemistry (Minor Elective, for students of other PG programmes)	2
	Total :	23
<u>Semester-III</u>		
CHM301	Molecular Spectroscopy (Core Paper)	3
CHM302	Biological Chemistry (Core Paper)	3
CHM303	Specialization Paper-I (A/I/O/P)*	3
CHM304	Specialization Paper-II (A/I/O/P)*	3
CHM305	Practical (A/I/O/P)*	6
CHM306-309	Elective Paper I (Any one out of the four papers) ⁺	3
CHM310M	Organic Chemistry - Applied Aspects Only (Minor Elective, for students of other PG programmes)	2
	Total :	23
<u>Semester-IV</u>		
CHM401	Computer Applications in Chemistry (core paper)	2
CHM402	Specialization Paper-III (A/I/O/P)*	2
CHM403	Specialization Paper-IV (A/I/O/P)*	2
CHM404	Specialization Paper-V (A/I/O/P)*	2
CHM405	Project	5
CHM406-409	Elective Paper II (Any one of the four papers) ⁺⁺	2
CHM410	Laboratory work for Computer Applications in Chemistry (Common to all branches)	1
	Total:	16
	Total :	80

A-Analytical Chemistry

I- Inorganic Chemistry

O-Organic Chemistry

P-Physical Chemistry

Elective Papers**+Elective – I**

CHM306	Forensic Analysis
CHM307	Chemical Applications of Group Theory
CHM308	Medicinal Chemistry
CHM309	Materials Chemistry

++Elective - II

CHM406	Environmental Chemistry
CHM407	Photo Inorganic Chemistry
CHM408	Bioorganic Chemistry
CHM409	Physical Methods in Chemistry

Minor Electives

To be offered by chemistry students from other PG programmes

* Details of specialization courses are given on the next page

* Details of Specialization Papers

Semester – III

Specialization Papers - I & II

		Credit
<u>Analytical Chemistry</u>		
CHM303 (A):	Principles of Analytical Chemistry	3
CHM304 (A):	Microanalytical Techniques	3
<u>Inorganic Chemistry</u>		
CHM303 (I):	Organometallic Chemistry of Transition Metals	3
CHM304 (I):	Bio-inorganic Chemistry	3
<u>Organic Chemistry</u>		
CHM303 (O):	Stereochemistry and Photochemistry	3
CHM304 (O):	Natural Products	3
<u>Physical Chemistry</u>		
CHM303 (P):	Electrochemistry	3
CHM304 (P):	Quantum Chemistry	3
<u>CHM305 Practical</u>		
CHM305 (A):	Analytical Chemistry Practical	6
CHM305 (I):	Inorganic Chemistry Practical	6
CHM305 (O):	Organic Chemistry Practical	6
CHM305 (P):	Physical Chemistry Practical	6

Semester – IV

Specialization Papers – III, IV, V

<u>Analytical Chemistry</u>		
CHM402 (A):	Separation Techniques	2
CHM403 (A):	Electroanalytical Methods	2
CHM404 (A):	Spectrochemical Analysis	2
<u>Inorganic Chemistry</u>		
CHM402 (I):	Structural Methods in Inorganic Chemistry	2
CHM403 (I):	Inorganic Rings, Chains, and Clusters	2
CHM404 (I):	Special Topics in Inorganic Chemistry	2
<u>Organic Chemistry</u>		
CHM402 (O):	Application of Spectroscopy to Structural Analysis	2
CHM403 (O):	Reagents and Organic Synthesis	2
CHM404 (O):	Heterocycles and Vitamins	2
<u>Physical Chemistry</u>		
CHM402 (P):	Statistical Mechanics	2
CHM403 (P):	Solid State Chemistry	2
CHM404 (P):	Chemical Kinetics	2
<u>CHM405: Project</u>		
CHM405 (A):	Analytical Chemistry	5
CHM405 (I):	Inorganic Chemistry	5
CHM405 (O):	Organic Chemistry	5
CHM405 (P):	Physical Chemistry	5

Semester-I

CHM 101: Analytical Chemistry-I

Credits: 3

1. **Introduction:** Scope & objectives, Analytical chemistry and chemical analysis, Classification of analytical methods, Method selection, Sample processing, Steps in a quantitative analysis, Quantitative range (bipartite classification), Data organisation, Analytical validations, Limit of detection and limit of quantitation, The tools of analytical chemistry and good lab practices.
2. **Analytical chemometrics:** Propagation of measurement uncertainties (inaccuracy and imprecision). Useful statistical test: test of significance, the F test, the student 't' test, the chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values, significant figures, regression analysis (least square method for linear and non-linear plots), statistics of sampling and detection limit evaluation. Chemometrics for optimization, modeling and parameter estimation, factor analysis, resolution and pattern recognition.
3. **Treatment of Equilibria:** Solvents and solutions, general treatment of equilibria in aqueous medium involving monoprotic weak acid and weak base, and salts of weak acids and weak bases. Activity and concentration, Effect of electrolytes on chemical equilibria, Calculation of pH, Constructing titration curves from charge balance and mass balance equations, Acid-base titrations and theory of pH indicators, Complexation equilibria and complexometric titrations, Redox equilibria and redox titration, Theory of redox indicators, Precipitation reaction and precipitation titrations and theory of adsorption indicators.
4. **Spectrophotometric Determination of Stoichiometry of Complexes:** Job's method of continuous variation, mole ratio and slope ratio analysis, Advantages and limitations, typical examples
5. **Automation in the Laboratory:** Principles of automation, Process control through automated instruments, Autoanalyzers (single channel and multi-channel), Basic sequences of multi-fold operational analyzers in segmented and non-segmented flows.

Books Recommended

1. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, *Modern Methods of Chemical Analysis*, 2nd Edition (1976), John Wiley, New York.
2. G. D. Christian, *Analytical Chemistry*, 5th Edition (1994), John Wiley & Sons, New York.
3. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Analytical Chemistry - An Introduction*, 7th Edition (2000), Saunders College Publishing, Philadelphia, London.
4. J. H. Kennedy, *Analytical Chemistry: Principles*, 2nd Edition (1990), Saunders Holt, London.

CHM:102 Inorganic Chemistry-I

Credits:3

1. **Metal-Ligand Bonding in Transition Metal Complexes:** Crystal field splitting diagrams in complexes of low symmetry; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions; experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory as applied to metal complexes, brief introduction to Angular Overlap Model.
2. **Electronic spectra of Transition Metal Complexes:** Spectroscopic ground states; Orgel energy level and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral Co(II) and

Ni(II) complexes and calculation of ligand-field parameters.

3. **Symmetry based concepts** of energy level diagrams of metal complexes. Symmetry elements and operations, determination of point group of a molecule, Group Representations, Features of specific character tables in reference to Orgel diagrams, Symmetry based concepts of Orgel energy level diagrams of metal complexes.

Books Recommended

1. F.A. Cotton and G. Wilkinson *Advanced Inorganic Chemistry*, 6th Edn. (1999), John Wiley & Sons, New York.
2. J.E. Huheey, E.A. Keiter and R.L. Keiter, *Inorganic Chemistry*, 4th Edn. (1993), Addison-Wesley Pub. Co., New York.
3. R. S. Drago, *Physical Methods in Inorganic Chemistry*, International Edn. (1971), Affiliated East-West Press, New Delhi.
4. Keith F. Purcell and John C. Kotz, *Inorganic Chemistry*, W. B. Saunders Com. (1987), Hong Kong.
5. K. Veera Reddy, *Symmetry and Spectroscopy of Molecules*, New Age International Pvt. Ltd., New Delhi (1999).
6. B.N. Figgis, *Introduction to Ligand Fields*, Wiley Eastern Ltd. New Delhi (1976).

CHM 103: Organic Chemistry-I

Credits: 3

1. **Aromaticity:** Benzenoid and nonbenzenoid systems, antiaromaticity, homoaromaticity, alternant and non-alternant hydrocarbons.
2. **Nucleophilic Substitution at Saturated Carbon:** Mechanism and Stereochemistry of SN1, SN2, SNi and SN2' reactions. Reactivity: The effect of substrate structure, attacking nucleophile, leaving group and reaction medium. Phase transfer catalysis and ultrasound, Ambient nucleophiles: Regioselectivity. Competition between SN1 and SN2 mechanisms.
3. **Neighbouring Group Participation:** Evidences of N.G.P.; the phenonium ion, participation by π and σ bonds, Anchimeric assistance. Classical versus non-classical carbonium ions—the present status.
4. *Protection and Deprotection of Functional Groups: protection of NH group, OH group, diols, carbonyl groups, carboxyl groups, double bonds and triple bonds.*
5. **Asymmetric Synthesis:** The chiral pool, chiral auxiliaries, enantiomeric excess, chiral catalysts and reagents.
6. **Synthesis in Action:** Mascalure, Salbutamol, Grandisol, Dofetilide.

Books recommended

1. Clayden, Greeves, Warren and Wothers, *Organic Chemistry*, Oxford University Press, 2001.
2. M.B. Smith & Jerry March, *March's Advanced Organic Chemistry*, 5th Edition (2001), John Wiley & Sons, New York.
3. Peter Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6th Edition (1997), Orient Longman Ltd., New Delhi.
4. S. M. Mukherjee and S.P. Singh, *Reaction Mechanism in Organic Chemistry*, 1st Edition (1990), Macmillan India Ltd., New Delhi.
5. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edition (1998), Addison – Wesley Longman Inc. (IS Edition)
6. G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis*, (2007), Freeman and Company, New York.
7. M. S. Singh, *Advanced Organic Chemistry: Reactions and Mechanism*: Pearson Education (Singapore) Pte. Ltd. (2005)

CHM 104: Physical Chemistry-I

Credits:3

1. **Electrochemistry:**
Metal/Electrolyte interface: OHP and IHP, potential profile across double layer region, potential difference across electrified interface; structure of the double layer: Helmholtz-Perrin, Gouy-Chapman, and Stern models.
Semiconductor (SC)/electrolyte interface: Creation of space charge region, capacity of space-charge, Mott-Schottky plots for n-type and p-type semiconductors, determination of flat-band potential and donor/acceptor densities, application of SC/electrolyte interface in solar cells.
 Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot, polarizable and non-polarizable interfaces.

2. **Chemical Kinetics:**
 Kinetics of complex reactions (reversible, simultaneous and consecutive), chain reactions; dynamic chain (Hydrogen-Bromine reaction, decomposition of ethane), branched chain (Hydrogen-Oxygen reaction), oscillatory reactions (Belousov-Zhabotinskii reaction), experimental techniques for fast reactions (stopped-flow, temperature- jump and flash photolysis).

3. **Surface Chemistry and catalysis:**
 Bimolecular surface reactions: reaction between a gas molecule and an adsorbed molecule, reaction between two adsorbed molecules, inhibition and activation energy of such reactions, catalytic activity at surfaces (volcano curve), transition state theory of surface reactions, rates of chemisorption and desorption, unimolecular and bimolecular surface reactions, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity.

Books Recommended:

1. Modern Electrochemistry, Vol. 2 A & B, J.O'M. Bockris and A. K. N. Reddy, 2nd Ed. Plenum Press, New York (1998)
2. Chemical Kinetics, K. J. Laidler, 3rd Ed. Harper & Row, New York (1987)
3. Physical Chemistry, P. W. Atkins, 8th Ed., Oxford University Press, New York,
4. Physical Chemistry, I.N. Levine, 5th Ed., Tata McGraw Hill Pub. Co. Ltd., New Delhi.

Practical

CHM105: Inorganic Chemistry Practical

Credits: 2

1. Quantitative separation and determination of the following pairs of metal ions using gravimetric and volumetric methods:
 - (i) Ag^+ (gravimetrically) and Cu^{2+} (Volumetrically)
 - (ii) Cu^{2+} (gravimetrically) and Zn^{2+} (Volumetrically)
 - (iii) Fe^{3+} (gravimetrically) and Ca^{2+} (Volumetrically)
 - (iv) Mg^{2+} (gravimetrically) and Ca^{2+} (Volumetrically)

2. Separation of a mixture of cations/anions by paper chromatographic technique using aqueous/non-aqueous media.

- (i) Pb^{2+} and Ag^+ (aqueous and non-aqueous media)
- (ii) Co^{2+} and Cu^{2+} (non-aqueous medium)
- (iii) Cl^- and I^- (aqueous-acetone medium)
- (iv) Br^- and I^- (aqueous-acetone medium)

CHM106: Organic Chemistry Practical

Credits: 2

1. Determination of neutralization equivalent of organic acids.
2. Separation and Identification of compounds having one or more functional groups

CHM107: Physical Chemistry Practical

Credits: 2

1. Saponification of ethyl acetate with sodium hydroxide by chemical method.
2. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
3. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
4. Distribution coefficient of I_2 between two immiscible solvents.
5. Conductometric titration of a weak acid with strong base.
6. Conductometric titration of a mixture of weak and strong acids.
7. Potentiometric titration of a strong acid with strong base using quinhydrone electrode.
8. Conductometric titration of KCl with AgNO_3 .
9. Molecular weight of a non-electrolyte by cryoscopy method.
10. Plateau of GM tube and study of counting statistics.

Semester-II

CHM201: Analytical Chemistry-II (Techniques in Analytical Chemistry)

Credits:3

1. **Polarography:** Origin of polarography, Current-voltage relationship, Theory of polarographic waves (DC and sampled DC (tast) polarograms), Instrumentation, Ilkovic equation, Qualitative and quantitative applications.
2. a. **Spectroscopic Techniques:** Theory, Instrumentation and applications of X-rays (emission, absorption, diffraction and fluorescence methods), Atomic absorption Spectroscopy, Atomic fluorescence spectrometry, Atomic emission spectrometry.
 b. **Molecular Spectroscopy:** UV-visible molecular absorption spectrometry (instrumentation and application), Molecular luminescence spectroscopy (fluorescence, phosphorescence, chemiluminescence).
3. **Separation Methods:** Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography, Gas chromatography, High-performance liquid chromatography
4. **Thermal Analysis:** Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods

Books Recommended

1. D.A. Skoog, *Principles of Instrumental Analysis*, 5th Edition (1998), Saunders College Publishing, Philadelphia, London.
2. G.W. Ewing, *Instrumental Methods of Chemical Analysis*, 5th Edition (1978), McGraw Hill Books Co., New York.
3. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, *Modern Methods of Chemical Analysis*, 2nd Edition (1976), John Wiley, New York.
4. J.H. Kennedy, *Analytical Chemistry: Principles*, 2nd Edition (1990), Saunders Holt, London.

CHM202: Inorganic Chemistry-II**Credits:3**

1. **Kinetics and Mechanism of Substitution Reactions:** Nature of substitution reactions; prediction of reactivity of octahedral, tetrahedral and square-planar complexes in terms of crystal field activation energy and structure preference energy; rates of reactions; acid hydrolysis, base hydrolysis and anation reactions.
2. **Electron Transfer Reactions:** Mechanism and rate laws; various types of electron transfer reactions, Marcus-Hush theory, correlation between thermal and optical electron transfer reactions; identification of intervalence transfer bands in solution.
3. **Metal Carbonyls and related compounds:** Preparation, structure, and properties: bonding in metal carbonyls, variants of CO bridging, vibrational spectra of metal carbonyls, principal reaction types of metal carbonyls.
4. **Optical Rotatory Dispersion and Circular Dichroism :** Basic Principles of ORD and CD techniques. ORD and Cotton effect, Faraday and Kerr effects; Applications in determining absolute configuration of metal complexes.

Books Recommended

1. F. Basalo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn (1967), Wiley Eastern Ltd., New Delhi.
2. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, 3rd Edn. (1999), ELBS, London.
3. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 6th Edn. (1999), John Wiley & Sons, New York.
4. D.N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, Universities Press (India) Ltd., Hyderabad (2001).
5. Keith F. Purcell and John C. Kotz, *Inorganic Chemistry*, W. B. Saunders Com. (1987), Hong Kong.
6. Martin L. Tobe and John Burgess, *Inorganic Reaction Mechanisms*, Longmans 1st Edn. (1999).

CHM203 Organic Chemistry-II**Credits:3**

1. **Addition to Carbon–Carbon Multiple Bonds:** Electrophilic, free-radical and nucleophilic addition: Mechanistic and Stereochemical aspects.
2. **Elimination reactions:** The E1, E2 and E1cB mechanisms, Orientation of the double bond. Hofmann versus Saytzeff elimination, Pyrolytic *syn*-elimination, Competition between substitution and elimination reactions
3. **Pericyclic Reactions:** Woodward-Hoffmann rules and molecular orbitals; Cycloaddition [2+2] and [4+2] and higher order reactions, 1,3-Dipolar cycloaddition and cheletropic reactions; Electrocyclic reactions. Sigmatropic rearrangements; Group transfer reactions: Ene reactions.
4. **Formation of Carbon-Carbon Bonds via Organometallic reagents:** Organocopper reagents, organozinc reagents, organoboron reagents, Palladium catalyzed coupling reactions.

5. **Synthetic Design:** Retrosynthetic analysis, Umpolung, Domino reactions, Functional group interconversion.

Books recommended

1. Clayden, Greeves, Warren and Wothers, *Organic Chemistry*, Oxford University Press, 2001.
2. M.B. Smith & Jerry March, *March's Advanced Organic Chemistry*, 5th Edition (2001), John Wiley & Sons, New York.
3. Peter Sykes, *A Guide Book to Mechanism in Organic Chemistry*, 6th Edition (1997), Orient Longman Ltd., New Delhi.
4. G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis*, (2007), Freeman and Company, New York.
5. S. M. Mukherjee and S.P. Singh, *Reaction Mechanism in Organic Chemistry*, 1st Edition (1990), Macmillan India Ltd., New Delhi.
6. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edition (1998), Addison – Wesley Longman Inc. (IS Edition).
7. S.M. Mukherjee and S.P. Singh, *Pericyclic Reactions*, MacMillan India, New Delhi.
8. Jagdamba Singh and L D S Yadav, *Advanced Organic Chemistry / Organic Synthesis*, Pragati Prakashan, 2011.
9. I. Fleming, *Pericyclic Reactions*, Oxford University Press, Oxford (1999).

CHM 204: Physical Chemistry-II

Credits: 3

1. **Corrosion:** Types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential), corrosion measurements (weight loss, OCP measurement, and polarization methods), passivity and its breakdown, corrosion prevention techniques (electrochemical, inhibitor, and coating methods).
Cyclic voltammetry: Instrumentation, current-potential relation applicable for Linear Sweep Voltammetry (LSV) and Cyclic Voltammetry (CV), interpretation of cyclic voltammograms and parameters obtainable from voltammograms.
2. **Micelles:** Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, thermodynamics of micellization, phase separation and mass action models, reverse micelles, solubilization.
Polymer: Molecular mass and its distribution, determination of molecular mass by osmometry, viscosity, light scattering and size exclusion chromatography methods, Glass transition temperature, the Flory-Huggins theory of polymer solutions, living radical polymerization, polymer nanocomposite.
3. **Equilibrium and Non- equilibrium Thermodynamics:**
Properties of non-ideal solutions, excess functions, Nernst heat theorem, third law of thermodynamics, variation of entropy with temperature, determination of absolute entropy of liquids and gases.
Entropy production in irreversible processes, fluxes and forces, coupled flows, linear phenomenological relations, Onsager's reciprocity relations, thermodynamic theory of membrane permeability, reverse osmosis.

Books Recommended

1. Modern Electrochemistry, J.O'M. Bockris and A. K. N. Reddy, Vol. 2 A & B, 2nd Edition, Plenum Press, New York (1998).
2. Electrochemical Methods: Fundamentals and Applications; A.J. Bard and L.R. Faulkner, 2nd Edition (2001), John Wiley & Sons, New York.
3. Micelles: Theoretical and Applied Aspects, Y. Moroi, Plenum Press, New York (1992).
Text Book of Polymer Science, F.W. Billmeyer Jr., 3rd Edition (1984), Wiley-Inter Science, New York.
4. Introduction of Thermodynamics of irreversible Processes, I. Prigogine.

CHM205: Chemical Binding**Credits: 3**

1. **Fundamental background:** Postulates and theorems of quantum mechanics, angular momentum, rigid rotor.
2. **The Schrödinger equation and its exact solutions:** The particle-in-a-box, Hydrogen atom, the variation theorem – Ritz variation principle.
3. **Atomic structure:** many electron wave functions, Pauli exclusion principle, Helium atom, atomic term symbols.
4. **Symmetry point groups:** Determination of point group of a molecule, representations, the great orthogonality theorem, character table, construction of character tables for c_{2v} and c_{3v} groups, symmetry adapted atomic basis sets, construction of molecular orbitals.
5. **Molecular structure:** Born-Oppenheimer approximation, molecular orbital treatment for H_2^+ , MO treatment of homo- and hetero nuclear diatomic molecules, Hückel MO treatment of simple and conjugated polyenes.

Books Recommended

1. Quantum Chemistry, I.N. Levine, 5th Edition (2000), Pearson Educ., Inc. New Delhi.
2. Physical Chemistry: A Molecular Approach, D.A. Mc Quarrie and J.D. Simon, (1998) Viva Books, New Delhi.
3. Valence Theory, J.N. Murrell, S.F.A. Kettle and J. M. Tedder, 2nd Edition (1965), John Wiley, New York.
4. Introductory Quantum Chemistry, A.K. Chandra, 4th Edition (1994), Tata Mcgraw Hill, New Delhi.

Practical**CHM206 : Inorganic Chemistry Practical****Credits: 2**

- 1 Preparation of coordination complexes and their characterization by magnetic susceptibility measurements and IR, UV / Vis, 1H NMR spectroscopic techniques.

CHM207 Organic Chemistry Practical**Credits: 2**

1. Preparation and characterization of two and three steps organic compounds.
2. Isolation of caffeine from tea leaves.

CHM208 Physical Chemistry Practical

Credits: 2

1. Rate constant of acid catalyzed hydrolysis of sucrose by polarimetric method.
2. Rate constant of acid catalyzed hydrolysis of sucrose by chemical method.
3. Rate constant of FeCl₃-catalyzed H₂O₂ decomposition by gasometric method.
4. Degree of hydrolysis of urea hydrochloride by kinetics method.
5. Equilibrium constant of KI + I₂ ⇌ KI₃ by distribution method.
6. Phase diagram of a binary organic system (Naphthalene and Diphenyl).
7. Determination of solubility and solubility product of sparingly soluble salt conductometrically.
8. Potentiometric titration of a redox system (ferrous ammonium sulfate with K₂Cr₂O₇).
9. Adsorption of acetic acid on charcoal to verify Freundlich adsorption isotherm. ?
10. Determination of half-life of a radionuclide.

CHM209 M : Polymer Chemistry

Credits: 2

1. **Introduction:** Classification of polymers, intermolecular forces in polymers.
2. **Mechanism and kinetics of step-growth and chain growth polymerization:** Radical, cationic, anionic and condensation polymerization, copolymerization, reactivity ratios, thermodynamic aspects of polymerization, mechanism of living radical polymerizations: nitroxide mediated polymerization (NMP), metal-catalyzed living radical polymerization, reversible addition-Fragmentation Chain Transfer (RAFT) radical polymerization, coordination polymerization, ring opening polymerization, click chemistry.
3. **Polymer solutions:** Flory-Huggins theory of polymer solutions, nature, size and shape of macromolecules in solution.
4. **Polymer structure and Physical properties:** Microstructure of polymer chains, crystallinity in polymers, glass transition temperature, rheological properties, molecular weight and its distribution.
5. **Specialty polymers:** Liquid crystalline polymers, conducting polymers, electroluminescent polymers, inorganic polymer, nanocomposites of polymers, biomedical polymers.

Books Recommended

1. Text Book of Polymer Science, 3rd Edition (1984), F. W. Billmeyer, Jr., Wiley-Interscience, New York.
2. Physical Chemistry, 8th Edition, P. W. Atkins, Oxford University Press, New York. **YEAR**
3. Principles of Polymerization, 3rd Edition (1991) G. Odian, John Wiley, Singapore
4. Principle of Polymer Sciences, P. Bahadur and N.V. Sastry, Narosa Publishing House, New Delhi (2002)
5. Polymer Sciences, V.R. Gowariker, N.V. Vishwanathan, J. Shreedhar , Wiley Eastern, New Delhi (1986)

Semester-III**CHM 301: Molecular Spectroscopy (Core Paper)****Credits: 3**

- 1. Introduction:** Interaction of electromagnetic radiation with matter, transition probability and selection rules, line-widths and line shapes, Fourier Transforms in spectroscopy.
- 2. Rotational and rotation-vibrational spectroscopy:** Microwave and Infrared spectroscopy of di- and polyatomic molecules, normal coordinates and their symmetry (CO₂), skeletal vibration and group frequency, FT-IR instrumentation.
- 3. Raman spectroscopy:** Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines.
- 4. Electronic spectroscopy:** Vibronic spectroscopy of diatomic molecules, Franck-Condon factor, dissociation and pre-dissociation, rotational fine structure, solvent effects. Photoelectron spectroscopy (PES): UV and X-ray PES of molecules.
- 5. Lasers and laser spectroscopy:** Principles of laser action, laser characteristics, pulsed lasers, laser cavity modes, Q-switching, mode locking, non-linear effects, harmonic generation, examples of lasers: He-Ne, Nd-YAG, titanium-sapphire., dye lasers. Lasers in spectroscopy: Raman, hyperRaman, CARS, femtosecond spectroscopy.
- 6. Single molecule spectroscopy:** Single molecule detection, confocal detection optics and configuration, applications.
- 7. Magnetic resonance:** A review of spin angular momentum, basic principles and relaxation times, intensity of NMR signals, electronic shielding, NMR in liquids: chemical shifts, spin-spin couplings, NMR spectra of AX, A₃X and AB systems. ESR of hydrogen, first order hyperfine energies, ESR of organic radicals in solution.
- 8. FT-NMR:** Rotating frame of reference, effect of RF pulses, FID, Multipulse operation, measurement of T₁ by inversion recovery method, spin echo and measurement of T₂, 2-D NMR, NMR hardware.

Books Recommended:

1. Modern Spectroscopy, J. M. Hollas, 4th edition (2004), John Wiley & Sons, Ltd., Chichester.
2. Introduction to Molecular Spectroscopy, G. M. Barrow, (1962) McGraw-Hill.
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. Mc Cash, 4th edition, (1994), Tata McGraw Hill, New Delhi.
4. Principle of Fluorescence Spectroscopy, L. R. Lakowicz, 3rd Edition, Springer. **YEAR?**
5. Introduction to Magnetic Resonance A. Carrington and A. D. Mc Lachlan, (1979), Chapman and Hall, London.
6. Nuclear Magnetic Resonance Spectroscopy, R. K. Harris, (1986), Addison Wesley, Longman Ltd, London

CHM 302: Biological Chemistry

(Core Paper)

Credits: 3

- 1. Molecules of life:** Amino acids and proteins, Carbohydrates-polysaccharides, lipids, cell-membranes and nucleic acids
- 2. Structure and function:** Protein structure, Ramachandran plot, protein folding: DNA/RNA structures, various forms (a, b, c, z) of DNA, t-RNA structure, transcription and translation, gene expression and DNA binding protein-zinc-finger protein.
- 3. Metabolism and Energetics:** Glycolysis , citric acid cycle , oxidative phosphorylation and transport through membranes
- 4. Enzyme kinetics, inhibition, drug action (selected examples)**
- 5. Metalloenzymes:** Hydrolytic and redox enzymes: Carbonic anhydrase and superoxide

dismutase

6. **Oxygen uptake proteins:** Hemerythrin and hemocyanin
7. **Molecular recognition:** Molecular organization, Chiral recognition and role of sugar in biological recognition

Books Recommended

1. L. Stryer, Biochemistry, 5th Edition, (2002) Freeman & Co. New York
2. D.L. Nelson and M.M. Cox, Lehninger Principles of Biochemistry 3rd Edition ((2002) McMillan North Publication
3. D. Voet, J. G. Voet, Biochemistry 3rd Edition (2004), Wiley International Publication.
4. I. Bertini, H. B. Gray, S. J. Lippard, J.S. Valentine, 1st South Asian Edn., (1998) Viva Books Pvt. Limited, New Delhi
5. M. B. Smith, Organic Synthesis, (1998) Mc Graw Hill Inc, New York

Specialization Papers I & II *Analytical Chemistry Specialization*

CHM 303 (A): Principles of Analytical Chemistry

Credits:3

1. **Acid-Base Equilibria:** General concept of acid-base equilibria in water and in non-aqueous solvent, Definition of pH and pH scale (Sorenson and operational definitions), and its significance, Hammett acidity function, pH calculation for aqueous solutions of very weak acid and very weak base, salts of weak acid and weak bases, mixture of weak acid and its salts, mixture of weak base and its salts, polybasic acids and their salts, polyamines and amino acid, composition of solution of polybasic acid as a function of pH, protolysis curves
2. **Buffer Solutions:** Theory of buffer solution, dilution and salts effects on the pH of a buffer, Buffer index, Criteria and expression of maximum buffer capacity, Application of pH buffers, Preparation of buffer solutions of known ionic strength (Typical examples). Practical limitations in use of buffers, Metal ion buffers and their applications, Biological buffers and their applications.
3. **Photometric Titrations:** Basic principles, comparison with other titrimetric procedures, types of photometric titration curves, Instrumentation (Titration cell, Detectors, choice of analytical wavelength). Quantitative applications, Typical examples of one component and multicomponent analyses.
4. **Chemical Sensors:** Principles, types of chemical sensors based on the modes of transductions, Types of chemical sensor based on the chemically sensitive materials (solid electrolyte, gas, semiconductor), Humidity sensors, Biosensors, Electrochemical sensors (Potentiometric sensors, Ion-selective electrodes, Membrane electrodes, Amperometric sensors, Clark and Enzyme electrodes).

Books Recommended

1. D.A. Skoog and D.M. West, *Fundamental of Analytical Chemistry*, International Edition, 7th Edition (1996), Saunders College Publishing, Philadelphia, Holt, London.
2. R.L. Pecsok, L.D. Shields, T. Cairns and L.C. McWilliam, *Modern Methods of Chemical Analysis*, 2nd (1976), John Wiley & Sons, New York.
3. D.A. Skoog, *Principles of Instrumental Analysis*, 5th Edition (1998), Saunders College of Publishing, Philadelphia, London.
4. H.A. Strobel, *Chemical Instrumentation: A Schematic Approach*, 2nd Edition (1973), Addison Wesley, Reading, Mass.

CHM 304(A): Microanalytical Techniques**Credits: 3**

1. General Introduction: Scope and objectives of microanalytical technique, Difference between micro and trace analysis, Microanalytical technique based on size and amount of the sample
2. Microanalysis of real-world Samples: Molecular recognition and targeted analysis using macrocyclic (crown ethers), macrobicyclic (cryptands), Supramolecular compounds (calixarenes) and polymeric materials
3. Biochemical Microanalysis: Estimation of carbohydrates, amino acids and ascorbic acid in biological systems, Estimation of protein in egg albumin, Estimation of free fatty acid, Iodine value and saponification value of fats/oils, Estimation of blood cholesterol, DNA and RNA
4. Inorganic microanalysis: Principle, Technique, qualitative and quantitative applications with special reference to Ring-oven technique and Ring colorimetric technique, Chemical microscopy
5. Organic Microanalysis: Determination of alkoxy, acetyl, acyl, hydroxyl, carbonyl, active hydrogen, nitroso, sulfonyl, amides and ester groups, Determination of molecular weight and percentage purity of carboxylic acid, Estimation of sugars, Estimation of unsaturation
6. Microanalysis by Kinetic Methods: Theoretical basis, Kinetic parameters, Kinetic methods of microanalysis: Tangent, fixed time and addition method

Books Recommended

1. P.L. Kirk, *Quantitative Ultramicroanalysis*, John Wiley.
2. C.L. Wilson and D.L. Wilson, *Comprehensive Analytical Chemistry*, Vol. I (A) and I(B), Elsevier.
3. G.D. Christian, *Analytical Chemistry*, John Wiley & Sons, New York (2001).
4. S.M. Khopkar, *Analytical Chemistry of Macrocyclic and Supramolecular Compounds*, Narosa Publishing House, New Delhi (2002).
5. Jag Mohan, *Organic Analytical Chemistry - Theory and Practice*, Narosa Publishing House, New Delhi (2003).

Inorganic Chemistry Specialization**CHM 303 (I): Organometallic Chemistry of Transition Metals****Credits: 3**

1. **Inorganic π -Acid Ligands:** Dioxygen and dinitrogen, nitrosyl, tertiary phosphines and arsines as ligands.
2. **Complexes of σ -donor ligands:** Transition metal alkenyls, alkynyls, carbenes and carbenes
3. **π -complexes of unsaturated molecules:** Preparation, bonding and structure of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis
4. **Transition metal compounds in catalysis:** Hydrogenation, hydroformylation and polymerization; Wacker Process
5. **Transition metal Compounds with M-H bonds:** Metal hydrides (classical and non-classical). Agostic interaction. Application of NMR in studying hydrido complexes

Books Recommended

1. F.A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 6th Ed. (1999) John Wiley & Sons, NY.

2. J.E. Huheey, Keiter and Keiter, Inorganic Chemistry, YEAR?
3. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, John Wiley. YEAR?
4. Ch. Elschenbroich and A. Salzer, Organometallics, VCH. YEAR?
5. J.P. Collman, L.S. Hegedus, J.R. Norton and R.G. Finke, Principles and Applications of Organotransition metal Chemistry, Univ. Sci. Books, Mill Valley. California. YEAR

CHM 304 (I): Bio-inorganic Chemistry

Credits: 3

1. **Role of alkaline earth metal ions in biological systems :** (i) Catalysis of phosphate transfer by Mg^{2+} ion, (ii) Ubiquitous regulatory role of Ca^{2+} in muscle contraction
2. **Iron, copper and molybdenum proteins with reference to their oxygenation and oxidase activity:** (i) Anti-oxidative functions: cytochrome P-450, catalases and peroxidases, (ii) Nitrate and nitrite reduction: NO_3 and NO_2 reductase, (iii) Electron transfer: cytochromes; blue copper proteins and iron-sulfur proteins and their Synthetic models, (iv) molybdo-enzymes – molybdenum cofactors : molybdenum-pterin? complexes, (v) Nitrogen fixation through metal complexation, nitrogenase, (vi) Photosynthesis (PS-I and PS-II).
3. **Metalloenzymes:** Urease, Hydrogenase, and Cyanocobalamine
4. **Interaction of metal complexes with DNA:** DNA probe and chemotherapeutic agents
5. **Iron storage and transport proteins:** Ferritin, Transferritin and Hemosiderin

Books Recommended

1. M. N. Hughes, *Inorganic Chemistry of Biological Processes*, 2nd Ed.(1981), John-Wiley & Sons, New York.
2. W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide*, Wiley, New York (1995).
3. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, (1994).
4. I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi (1998)

Organic Chemistry Specialization

CHM 303 (O): Stereochemistry and Photochemistry

Credits: 3

1. **Stereochemistry:** Enantioselective synthesis with chiral non racemic reagents and catalysts: Hydroboration with chiral boranes ($I_{PC}BH_2$), $(I_{PC})_2BH$, Carbonyl group reduction with chiral complex hydride (BINAL-H, Chiral oxazaborolidines), Chiral organometal complex $-(-)DAIB$; 3-exo-dimethylamino isoborneol. Enantioselective epoxidation of alkene: Sharpless epoxidation, enantioselective hydrogenation with $[Rh(DIPAMP)]^+$. Diastereoselective synthesis: Aldol reactions (Chiral enolate & Achiral Aldehyde and Achiral enolate and chiral aldehyde). **Optical** Activity in absence of chiral carbon: biphenyls and Allenes and Atropisomerism.
2. **Conformation:** Conformational analysis of decalines and cyclohexene.
3. **Photochemistry:**
 - (a) **Introduction and Basic Principles of Photochemistry:** Absorption of light by organic molecules, properties of excited states, mechanism of excited state processes and methods of preparative photochemistry.
 - (b) **Photochemistry of alkenes and related compounds:** Isomerization, Di- π -methane rearrangement and cycloadditions.
 - (c) **Photochemistry of aromatic compounds:** Ring isomerization and cyclization reactions.

(d) Photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic and α , β and β , γ unsaturated carbonyl compounds, Norrish type-II cleavage. Hydrogen abstraction: Intramolecular and intermolecular hydrogen abstraction, photoenolization. Photocyclo-addition of ketones with unsaturated compounds: Paterno-Buchi reaction, photodimerisation of α , β -unsaturated ketones, rearrangement of enones and dienones, Photo-Fries rearrangement

4. **Rearrangements:** Sommelet-Hauser, Favorskii, rearrangements. Hofmann-Löffler-Freytag reaction, Barton reaction and Shapiro reaction.

Books Recommended

1. M.B. Smith and J. March, *March's Advanced Organic Chemistry-Reactions, Mechanisms and Structure*, 5th Edition (2001), John Wiley & Sons, New York.
1. D. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edition (1994), Wiley Eastern Ltd., New Delhi.
2. J. Aube and R. E. Gawley, *Principles of Asymmetric Synthesis*. YEAR
3. E.L. Eliel, S.H. Wilen and L.N. Mander, *Stereochemistry of Organic Compounds*, Wiley Interscience, New York (2004).
4. Paul de Mayo, *Molecular Rearrangements*, Vol.I & II, Interscience Publishers, New York (1963).
5. John D. Coyle, *Introduction to Organic Photochemistry*, John Wiley and Sons, New York (1986).
6. C.H. Depuy and O.L. Chapman, *Molecular Reactions and Photochemistry*, 2nd Edition (1988), Prentice-Hall of India (P) Ltd., New Delhi.
7. F.A. Carey and R.J. Sundberg, *Photochemistry in Advanced Organic Chemistry*, Chapter 13, Part A, 3rd Edition (1990), Plenum Press, New York.
8. N. J. Turro, *Modern Molecular Photochemistry*, University Science Books, Sausalito (1991).

CHM 304 (O): Natural Products

Credits: 3

1. **Alkaloids:** Structure elucidation of alkaloids – a general account; Structure, synthesis, and stereochemistry of Narcotine and Quinine; synthesis and stereochemistry of Morphine, Lysergic acid and Reserpine.
2. **Terpenoids:** Camphor, Longifolene*, Abietic acid, and Taxol.
3. **Steroids:** Cholesterol
4. **Prostaglandins and Thromboxanes :** Introduction, nomenclature of prostaglandins and thromboxanes; approaches to prostaglandin synthesis; cyclohexane precursors (Woodward synthesis of PGF_{2a}), bicycloheptane precursors (Corey's synthesis of prostaglandins E and F)
5. Retrosynthetic analysis of morphine and Reserpine and Longifolene.

* **Synthesis only.**

Books Recommended

1. Nitya Anand, J.S. Bindra and S. Ranganathan, *Art in Organic Synthesis*, 2nd Edition (1970), Holden Day, San Francisco.
2. S.W. Pelletier, *Chemistry of the Alkaloids*, Van Nostrand Reinhold Co., New York (1970).
3. K.W. Bentley, *The Alkaloids*, Vol. I., Interscience Publishers, New York (1957).
4. I. L. Finar, *Organic Chemistry*, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi
5. J.W. Apsimon, *Total Synthesis of Natural Products*, Vol. 1-6, Wiley-Interscience Publications, New York (Vol. 1, 1973).
6. J.S. Bindra and R. Bindra, *Creativity in Organic Synthesis*, Academic Press, NY (1975).
7. J.S. Bindra and R. Bindra, *Prostaglandins Synthesis*, Academic Press. Inc., New York, London (1977).
8. K. C. Nicolaou, *Classics in Total Synthesis of Natural Products*, Vol. I (1996) & Vol. II (2003).
9. J. Clayden, N. Greeves, S. Warren, and P. Wothers, *Organic Chemistry, Chapter 30*, Oxford University Press, Oxford (2001).

Physical Chemistry Specialization
CHM 303 (P): Electrochemistry

Credits: 3

1. **Activity coefficient and ionic migration in electrolyte solutions:** Quantitative treatment of Debye- Hückel theory of ion-ion interaction and activity coefficient, applicability and limitations of Debye-Hückel limiting law, its modification for finite-sized ions, effect of ion-solvent interaction on activity coefficient. Debye-Hückel-Onsagar (D-H-O) theory of conductance of electrolyte solution, its applicability and limitations. Pair-wise association of ions (Bjerrum and Fuoss treatment), modification of D-H-O theory to account for ion-pair formation, determination of association constant (K_A) from conductance data.
2. **Electrical double layer at metal/electrolyte interface:** Thermodynamics of double layer, electrocapillary equation, determination of surface excess and other electrical parameters-electrocapillarity, excess charge capacitance, and relative surface excesses. Metal/ water interaction-contact adsorption, its influence on capacity of interface, complete capacity-potential curve, constant capacity region hump. Specific adsorption.
3. **Electrode kinetics:** Multistep reactions- a near equilibrium relation between current density and over potential, Concept of rate determining step. Determination of reaction order, stoichiometric number, and transfer coefficient. Electrocatalysis-comparison of electrocatalytic activity. Importance of hydrogen evolution reaction and its mechanism.
4. **Electrochemical techniques:** Impedance technique-its application for studying electrode kinetics and corrosion. Rotating disc electrode (RDE): Application of measurement of electrochemical rate constant.

Books Recommended

1. *Modern Electrochemistry*, Vol. 1 & 2A and 2 B, J.O'M. Bockris and A.K.N. Reddy, Plenum Press, New York (1998).
2. *Electrochemical Methods: Fundamentals and Applications*; A.J. Bard and L.R. Faulkner, 2nd edition (2001), John Wiley & Sons, New York.

CHM 304 (P): Quantum Chemistry

Credits: 3

1. **Fundamentals:** Review of classical mechanics, general formulation of quantum mechanics, review of angular momentum, harmonic oscillator problem.
2. **Approximation methods:** Stationary perturbation theory for non-degenerate and degenerate systems with examples, time-dependent perturbation theory, radiative transitions, Einstein coefficients.

3. **Many Electron atoms:** Electron correlation, addition of angular momenta, Clebsch-Gordan series, total angular momentum and spin-orbit interaction.
4. **Group Theory:** Review and applications.
5. **Ab initio methods for closed shell systems:** Review of molecular structure calculations, Hartree-Fock SCF method for molecules, Roothaan-Hartree-Fock method, selection of basis sets. Density functional method: energy as a functional of charge density, Kohn-Sham equations.

Books Recommended

1. *Molecular Quantum Mechanics*, P.W. Atkins and R.S. Friedman, 3rd edition (1997), Oxford University Press. Oxford.
2. *Quantum Chemistry*, H. Eyring, J. Walter and G.E. Kimball, (1944) John Wiley, New York.
3. *Quantum Chemistry*, I.N. Levine, 5th edition (2000), Pearson Educ., Inc., New Delhi.
4. *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure*, A. Szabo and N. S. Ostlund, (1982), Dover, New York.

Practicals

CHM 305 (A): Analytical Chemistry Practical

Credits: 6

1. Determination of ferrous ammonium sulfate potentiometrically with standard ceric sulfate solution (Direct and back titration).
2. Determination of concentration of halide ion(s) in the given solution potentiometrically.
3. Conductometric titration of (i) strong acid, monobasic weak acid or polybasic weak acid with strong base (ii) zinc with EDTA, and (iii) KCl vs AgNO₃
4. To obtain the protolysis curves involving cases of weak acid, mixture of acids and polybasic acid employing a pH meter and determine the amount of the respective acid (in ppm) in the given solution
5. Determination of Na₂CO₃ content (in %) of washing soda using a pH meter
6. Analysis of mixture of carbonate and bicarbonate (percent in ppm range) using a pH meter or suitable indicators
7. To study the current-potential characteristics of Cd²⁺ ions using DC polarography, sampled DC, cyclic voltammetry and pulse polarographic techniques
8. Determination of Cd²⁺ ions concentration in given solution polarographically following (i) calibration (ii) standard addition and (iii) the pilot-ion procedures
9. Determination of Zn²⁺ ions present at the ppm level in the solution employing conventional D.C. and pulse polarographic techniques
10. Determination of trace metal impurities present in a polluted water sample by anodic stripping voltammetric procedure
11. **Statistical Treatment of Results**
 1. Determination of accuracy, precision, mean deviation, standard deviation, coefficient of variation, normal error curve and least square fitting of certain set of experimental data in an analysis.
 2. Composition of two sets of results in terms of significance (Precision and accuracy) by (i) student's t-test, (ii) F-test

12. Solvent Extraction: Determination of Fe (III) by chloride extraction in ether
13. Complexometric and Redox Titrations
 1. Metal-EDTA titrations using Eriochrome Black T, Xylenol orange and PAN indicators (only back titration or substitution titration methods).
 2. Estimation of the purity of oxalic acid employing standard Ce (IV) solution.
14. Spectrophotometric Analysis
 1. Spectrophotometric determination (in ppm) of Fe (II) or Fe(III) using 1,10 Phenanthroline (or thiocyanate) as colorimetric reagent.
 2. Colorimetric determination of chromium (VI) (in ppm) using 1,5 diphenyl carbazide as a reagent for colour development
15. Quantitative analysis of APC tablet by NMR or IR spectroscopy
16. Water Analysis: Analysis of water samples for the following parameters
(I) BOD, (ii) COD, (iii) Dissolved oxygen, (iv) total phosphorous, (v) sulfur as SO₂, (vi) total hardness and chloride, (vii) total dissolved solids.
17. To prepare a buffer solution of known ionic strength and to find its maximum buffer capacity

CHM 305(D):Inorganic Chemistry Practical

Credits: 6

1. (a) Synthesis and structural characterization (IR, electronic spectra and magnetic susceptibility) of [Ni(py)₄(NCS)₂].
(b) Synthesis of a series of Ni(II) complexes (with ligands of varying ligand field strength), electronic spectral interpretation and calculation of various ligand-field parameters.
 2. Synthesis and structural characterization (IR, Electronic spectra) of the *cis*- and *trans*-isomers of [Co(en)₂Cl₂]
 3. Synthesis and characterization (IR and PMR & CMR) of [Al(acac)₃]
-
1. Synthesis, purification by sublimation and structural characterization (IR and electronic spectra) of ferrocene.
 2. Acetylation of ferrocene and separation of the acetyl derivative by column chromatography.

CHM305(O): Organic Chemistry Practical

Credits: 6

1. Separation and identification of organic mixtures containing up to three components.
2. Preparation of organic compounds involving several stages, characterization of intermediates and final products by IR and NMR spectroscopy.
3. Techniques of organic chemistry: Special practical's involving steam distillation, photo-isomerization and thin layer chromatography etc.
4. Quantitative analysis of (i) sulphur and (ii) nitrogen.

CHM305 (P): Physical Chemistry Practical*Credits: 6*

1. Kinetics of decomposition of benzene diazonium chloride.
2. Conductometric study of the kinetics of saponification of ethyl acetate.
3. Determination of transport numbers of Cu^{2+} and SO_4^{2-} by Hittorf's method.
4. Conductometric titration of triple mixture ($\text{HCl} + \text{NH}_4\text{Cl} + \text{KCl}$) with (i) NaOH and (ii) AgNO_3 .
5. Analysis of halide mixture by differential potentiometry.
6. Conductometric titration of a polybasic acid.
7. Verification of the Nernst law of electrode potential.

Determination of band-gap of a semiconductor.

Ternary phase diagram of water, benzene, and acetic acid.

Determination of molecular weight of a macromolecule by viscometry.

Half-life periods of a source containing two radionuclides.

Absorption coefficient of metal absorbers for ^{60}Co γ - rays.

Electrochemical Impedance study of metal/solution interface.

Cyclic Voltammetry of the $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$ system.

Corrosion study of steel in an acid solution.

Elective Papers**Elective-I (Group A)****CHM 306: Forensic Analysis***Credits: 3*

1. **Introduction:** Profile of a forensic laboratory, Forensic Scientists' role and quality control, Crime-scene investigation, Collection and preserving physical evidences and evidentiary documentation, Future prospects of forensic analysis
2. **Real Case Analysis:** Liquor analysis, Trap-case analysis, Petroleum product analysis, Fire and Debris analysis, Injuries, Firearm wounds, Asphyxia and stress analysis (only analytical identifications).
3. **Forensic Toxicology:** Analysis of various types of poisons (corrosive, irritant, analgesic, hypnotic, tranquillizer, narcotic, stimulants, paralytic, anti-histamine, domestic and industrial (gaseous and volatile) poisoning and food poisonings), Explosive and explosion residue analysis, Lethal drug analysis (sampling, sealing, packing, laboratory methods of testing, reporting the analysis results, court evidence and medico-legal aspects for the consideration of chemical data as a proof for crime), Importance of physiological tests in forensic toxicology
4. **Instrumentation for Forensic Analysis**
5. (a) **Physical, Biological and Chemical Methods:** Non-destructive testing probes including radiography, Xera-radiography, Surface penetrations method (SEM and Laser Probes), Fluoroscopy, Clinical methods: ELISA, RIA and immunodiffusion, analysis of glucose, bilirubins, total cholesterol, creatinine, blood urea nitrogen and barbiturates in biological fluids, DNA-finger printing, Examination and grouping of blood strains and seminal strains, Data retrieval and automation techniques for forensic examination with reference to presence of drugs, glasses, paints, oils and adhesives at crime spot.

(b) **Instrumental Methods:** Sample preparation, calibration of instruments for accuracy and reproducibility of results in forensic analysis, method validation technique and requirements, procurement of standard samples, Forensic applications of TLC, HPTLC, HPLC, GC, FT-IR, AAS, GC-MS, UV-visible spectrophotometer with emphasis over standard operational procedures (SOPs) for test samples.

Books Recommended

1. W.J. Welcher (Ed.), *Scott's Standard Methods of Chemical Analysis*, Vol. III A, 6th Edition (1966), and vol. III B, 5th Edition (1975), Van Nostrand Reinhold Co. London.
2. Peter Fordham, *Non-destructive Testing Techniques*, 1st edition (1968), London Business Publications Ltd., London
3. W. Horwitz, *Official Methods of Analysis*, 11th Edition (1970), Association of Official Analytical Chemists, Washington DC.
4. K. Simpson and B. Knight, *Forensic Medicine*, 9th Edition (1985), Edward Arnold Publishers Ltd., London.

CHM 307: Chemical Applications of Group Theory**Credits: 3**

1. **Group Theory in Chemistry:** Classification of Groups; Matrix representation of symmetry elements and point groups, matrices of C_{3v} and C_{4v} point groups, transformation matrices; Structure of character tables, determination of symmetry species for translations and rotations.
2. **Chemical Applications of Group theory**
 - (i) **IR and Raman Spectroscopy:** Brief introduction to molecular vibrations; selection rules for fundamental vibrational transitions, symmetry of normal modes of molecules, Infrared and Raman activity of some typical molecules (molecules of C_{2v} , C_{3v} , C_{4v} , D_{2h} , D_{3h} , D_{4h} , T_d and O_h point groups)
 - (ii) **Crystal Field Theory:** Splitting of levels and terms in chemical environment, construction of energy level diagrams, selection rules and polarizations.
 - (iii) **Molecular Orbital Theory:** Introduction, transformation properties of atomic orbitals; hybridization schemes for σ - and π -bonding, hybrid orbitals as LCAOs; Molecular Orbital Theory for some typical AB_n types ($n = 2, 3, 4, 6$) of molecules (H_2O , NH_3 and BH_3)
 - (iv) **Electronic Spectra:** General considerations, typical examples from tetrahedral and octahedral systems, Orgel energy level diagrams.

Books Recommended

1. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn. (1999), John Wiley & Sons, New York.
2. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 2nd Edn. (1999), Prentice Hall International Inc., London.
3. K. Veera Reddy, *Symmetry and Spectroscopy of Molecules*, New Age International Pvt. Ltd., New Delhi (1999).

CHM308 : Medicinal Chemistry**Credits: 3**

1. **Structure and activity:** Relationship between chemical structure and biological activity (SAR). Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery.
2. **Drugs based on a substituted benzene ring:** Chloramphenicol, salmeterol, tolazamide, diclophenac, tiapamil, intryptyline

3. **Drugs based on five-membered heterocycles:** Tolmetin, spirapril, oxaprozine, sulconazole, nizatidine, imolamine, isobuzole.
4. **Drugs based on six-membered heterocycles :** Warfarin, quinine, norfloxacin and ciprofloxacin, methylclothiazide, citrine, terfenadine.
5. **Drugs based on seven-membered heterocyclic rings fused to benzene:** Chlordiazepoxide, diazepam, diltiazem.
6. **Drugs based on heterocycles fused to two benzene rings:** Quinacrine, tacrine,
7. **β -Lactam antibiotics:** Penicillin, cephalosporin.
8. **Drugs based on five-membered heterocycles fused to six-membered rings:** Acyclovir, methotrexate.
9. **New Chemical Entities as Clinical agents**
Synthetic: Ritonavir, erbumine
Natural: Hamamelitannin, pinophilin A & B

Books Recommended

1. A. Burger, *Medicinal Chemistry*, Vol. I-III, (1995) Wiley Interscience Publications, New York.
2. W. O. Foye, *Principles of Medicinal Chemistry*, 3rd Edition (1989), Lea & Febiger/Varghese Publishing House, Bombay.
3. D. Lednicer and L. A. Mitscher, *The Organic Chemistry of Drug Synthesis*, (1977) Vol. I-III, Wiley Interscience.
4. A. Kar, *Medicinal Chemistry*, (1993) Wiley Eastern Ltd., New Delhi.
5. N. K. Terrett, *Combinatorial Chemistry*, (1998) Oxford Univ. Press, Oxford.
6. Daniel Lednicer *Strategies for organic drug synthesis and design* (2009), John Wiley & Sons, New York.

CHM 309 Materials Chemistry

3 Credits

1. **Introduction:** Materials and their classification, inorganic and organic materials.
2. **Inorganic materials:** Design and synthesis of inorganic materials, requirements and constraints, combination properties of composites, functional materials, active materials; solid state reactions for synthesis of inorganic materials: ceramic methods, precursor method and sol-gel synthesis, physical and chemical vapour depositions; carbides, nitrides, structural and functional ceramics, intermetallics; intrinsic and extrinsic properties: electrical, optical and magnetic properties; ceramic superconductors, magnetic ceramics.
3. **Organic materials:** Molecular electronics: molecular materials for electronics and molecular scale electronics: Molecular properties, molecular arrangement and molecular interactions, piezoelectric and pyroelectric organic materials; molecular magnets based on transition metal complexes and organic ferromagnets, organic non-linear optical materials: photochromic organic materials and their classes; conducting polymers: polyacetylene, polypyrrole, polyaniline and polythiophene; conductive charge transfer materials: TTF-TCNQ, metal-dithiolate systems, fullerenes. Langmuir-Blodgett films, molecular electronic logic and architectures.

Textbooks

1. P.J. Vander Put, *Inorganic Chemistry of Materials*, Plenum Press, New York, 1998.
2. M.C. Petty, M.R. Bryce and D. Bloor, Editors *An Introduction to Molecular Electronics*, Edward Arnold, London 1995.

CHM-310M : Organic Chemistry-Applied Aspects**Credits:3**

1. **Organic chemistry and industry**
2. **Life begins with nucleic acids.** Sugar alcohols, *S*-glycosides. vitamin-C and inositols
3. **Brief introduction of the following with context to life:** Aspirin, adrenaline, coniine, thujone, cholesterol, prostaglandins, penicillines.
4. **Crixivan**-organic Chemists' answer to HIV.
5. **Bio-polymers:** polysaccharides - starch, cellulose, sucrose, amino acids and polypeptides, proteins.
6. **Synthetic polymers:** properties and uses - Polyester, poly-tetrafluoroethylene, polyamino acids, polycyanoacrylates, polyurethanes, silicone rubbers, polymeric antioxidants, polyphosphazenes, divinylether - maleic anhydride cyclopolymer (DIVEMA)

Books Recommended

1. Yescombe, Sources of information on rubber, plastic and allied industries, Pergamon Press, 1968.
2. Peter Bernfeld, Biogenesis of Natural compounds, 2nd edition, Pergamon press, 1967.
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic chemistry, Oxford University press INC, New York, 2001
4. Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd edition, Pearson Prentice Hall, 2005

Semester-IV**CHM 401: Computer Applications in Chemistry (Core Paper)****Credits: 2**

- 1 **FORTRAN Programming:** Types of Constants and Variables in Fortran, Dimension, Data, Type, COMMON and EQUIVALENCE statements, Arithmetic and Logical IF, IF-THEN-ELSE constructs, 'DO' statement, Various types of 'I/O' statements, Library functions, Statement functions, Function subprograms and subroutine subprograms.
- 2 **Numerical Methods:** Roots of Polynomials, Solution of Linear simultaneous equations, matrix multiplication and inversion. Numerical integration. Statistical treatment of data, variance and correlations.

Books Recommended

1. V. Rajaraman, *Fortran 77*, Prentice Hall (India), New Delhi (1997)
2. C. Xavier, *Fortran 77 and Numerical Methods*, New Age International Pvt. Ltd. Publishers, New Delhi (1994)
3. S. Lipschutz and A. Poe, Schaum's Outline Series – Theory and Problems of Programming with Fortran including structured Fortran, Mc Graw Hill Book Company, Singapore (1982)
4. K. V. Raman, *Computers in Chemistry*, Tata McGraw Hill (1993). [Reference book]

Specialization Papers***Analytical Chemistry Specialization*****CHM 402 (A): Separation Techniques****Credits: 2**

1. **Separation Techniques Based on Phase Equilibria:** Process optimization, Resolution (Fundamental equation). Distillation: Fractional distillation, Molecular distillation.

Chromatography: Gas chromatography, high performance liquid chromatography, Ion chromatography, Size exclusion chromatography, HPTLC, Bonded phase chromatography (BPC), Super critical fluid chromatography (SFC). Solvent Extraction: Liquid-Liquid and super critical fluid extraction, Sublimation: Normal and vacuum sublimation. Crystallization: Zone refining and Fractional crystallization.

2. **Separation Techniques Based on Rate Processes:** (a) Barrier-separation methods: Membrane separation-Ultra-filtration, dialysis, electro-dialysis, electro-osmosis, reverse osmosis(b) Field separation methods: Electrophoresis, Ultracentrifugation

Books Recommended

1. G.H. and H. Freiser, *Solvent Extraction in Analytical Chemistry*, 1st Edition (1958), John Wiley, New York.
2. B.L. Karger, L.R. Snyder and C. Howarth, *An Introduction to Separation Science*, 2nd Edition (1973), John Wiley, New York.
3. E.W. Berg, *Chemical Methods of Separation*, 1st Edition (1963), McGraw Hill, New York.
4. D.G. Peters, J.M. Hayes and C.M. Hieftj, *Chemical Separation and Measurements*, 2nd Edition (1974), Saunders Holt, London.
5. J.D. Seader and E.J. Henley, *Separation Process Principles*, 1st Edition (1998), John Wiley & Sons. Inc., New York.

CHM 403 (A): Electroanalytical Methods

Credits: 2

1. **General Introduction:** Electrocapillary curve and electrocapillary maximum potential, Mercury electrodes (DME, SME, HMDE), Rotating platinum electrode. Three-electrode system.
2. **Polarography:** Origin of polarography, Interpretation of a polarographic curve. Instrumentation. Limiting current, residual and charging current, diffusion current, migration current. Supporting electrolytes. Effect of supporting electrolyte on the limiting current. Diffusion coefficient and its evaluation. Ilkovic equation, its derivation and applications. Estimation of n-value(s). Theory and equations of different current-potential curves. Criteria of polarographic reversibility. Quasi-reversible and irreversible processes. Half-wave potentials and their significance. Interpretation of catalytic, kinetic, adsorption and capacitive currents. Polarographic maxima and maximum suppressors. Methods of quantitative analysis: absolute, comparative and the PILOT ION methods.
3. **Modern Polarography:** Necessity and development of new voltammetric techniques and their comparison with classical polarography. Fundamentals of sampled DC polarography (Test), oscillography, differential and derivative voltammetry, cyclic, pulse, alternating current and square wave polarography.
4. **Related Techniques:** Amperometric titration, Chronoamperometry, Chronopotentiometry. Controlled-potential and constant current coulometry. Stripping analysis.

Books Recommended

1. L. Meites, *Polarographic Techniques*, 2nd Edition (1965), John Wiley, New York.
2. J. Heyrovsky and K. Kuta, *Principles of Polarography*, 1st Edition (1966), Academic Press, New York.
3. D.A. Skoog, F.J. Holler and T.A. Nieman, *Principles of Instrumental Analysis*, 5th Edition (1998), Saunders College Publishing, Harcourt Brace & Company, U.S.A.
4. A.J. Bard and L.R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, 2nd Edition (2000), Wiley, New York.

Additional References

1. I.M. Kolthoff and J.J. Lingane, *Polarography*, 2nd Edition (1952), Wiley Intersciences, New York.
2. C.W.C. Milner and G. Phillips, *Coulometry in Analytical Chemistry*, Pergamon Press, New York (1967).

CHM 404 (A): Spectrochemical Analysis***Credits: 2***

1. **Nuclear Magnetic Resonance Spectroscopy:** Theory of nuclear magnetic resonance, Applications of ¹H NMR, ¹³C, ³¹P NMR, Quantitative applications of NMR: Drug Analysis, Molecular Weight determination.
2. **Electron Spin Resonance Spectroscopy:** Theory, Instrumentation and Important analytical applications
3. **Electron Spectroscopy:** Theory, Instrumentation and applications of Electron spectroscopy (XPS, XRF and Auger),
4. **Plasma Emission Spectroscopy:** Theory. Instrumentation and Analytical applications of inductively coupled plasma emission spectroscopy (ICPE).
5. **Applications in analysis of special materials:** Analysis of dairy products and petrochemicals

Books Recommended

1. D.A. Skoog, F.J. Holler and T.A. Nieman, *Principles of Instrumental Analysis*, 5th Edition (1998), Harcourt Brace & Company, Florida.
2. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, *Modern Methods of Chemical Analysis*, 2nd Edition (1976), John Wiley, New York.
3. J.M. Hollas, *Modern Spectroscopy*, 3rd Edition (1996), John Wiley, New York.
4. H.A. Strobel, *Chemical Instrumentation – A Systematic Approach*, 2nd Edition (1973), Addison Wesley, Mass.
5. D.C. Garratt, *the Quantitative Analysis of Drugs*, 2nd Edition (1992), Chapman and Hall Ltd., London.
6. W. Horwitz (Editor), *Official Methods of Analysis*, 11th Edition (1970), Association of Official Analytical Chemists, Washington DC.

Inorganic Chemistry Specialization

CHM 402 (I): Structural Methods in Inorganic Chemistry

Credits: 2

NMR Spectroscopy: (i) Use of Chemical shifts and spin-spin couplings for structural determination, (ii) Double resonance, and Dynamic processes in NMR, (iii) Decoupling phenomenon, Nuclear Overhauser Effect, DEPT spectra and structural applications in ^{13}C NMR, (iv) Use of Chemicals as NMR auxiliary reagents (shift reagents and relaxation reagents) (v) ^1H NMR of paramagnetic substances. (vi) NMR of Metal nuclei.

Electron Spin Resonance Spectroscopy: Basic principle, Hyperfine Splitting (isotropic systems); the g -value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Electron-electron interactions, anisotropic effects (the g -value and the hyperfine couplings); Structural applications to transition metal complexes.

Vibrational Spectroscopy: Applications of vibrational spectroscopy in investigating the stretching and bending modes of molecules (AB_3 and AB_4 types).

Books Recommended

1. E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, *Structural Methods in Inorganic Chemistry*, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.
2. R. S. Drago, *Physical Methods in Chemistry*, International Edition (1992), Affiliated East-West Press, New Delhi.
3. R. S. Drago, *Physical Methods in Inorganic Chemistry*, 1st Edn.(1971), Affiliated East-West Press, New Delhi.
4. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, 4th Edn. (1986), John Wiley & Sons, New York.
5. W. Kemp, *Organic Spectroscopy*, 3rd Edn. (1991), Macmillan, London.
6. G. Aruldas, *Molecular Structure and spectroscopy*, Prentice Hall of India Pvt. Ltd., New Delhi (2001).

CHM 403 (I) Inorganic Rings, Chains, and Clusters

Credits: 2

1. Clusters and element-element bonds: Polyhedral boranes: Electron deficiency vs sufficiency. Types and IUPAC nomenclature. Wade's polyhedral skeleton electron pair theory (PSEPT). W. N. Lipscomb's styx rules and semi-topological structures of boranes. Equivalent and resonance structures. Wade's vs Lipscomb's methods of studying higher boranes.

2. Heteroboranes: Types of heteroboranes with special reference to carboranes, structure, bonding and IUPAC nomenclature. Metallaboranes, Metallacarboranes, metal σ and μ bonded borane/carborane clusters. Resemblance of Metallaboranes/ Metallacarboranes with ferrocene and related compounds. Applications of Metallaboranes/Metallacarboranes as drug delivery system. Applications of PSEPT over heteroboranes.

3. Principle of Isolobility: Development and formulation of the concept of isolobility and its applications in the understanding of structure and bonding of heteroboranes.

4. Metal Clusters: Metal-metal bonds. Concept of quadrupolar bond and its comparison with a C-C bond; Types of metal clusters and multiplicity of M-M bonds. Simple and condensed metal carbonyl clusters. Applications of PSEPT and Wade's-Mingo's and Lauhr's rule over metal carbonyl clusters. Metal halide and metal chalcogenide clusters: Bloomington schuffle in dinuclear tungsten clusters.

5. Heteropoly and Isopoly acids: Structural principles and their applications

6. Inorganic Polymers: Classification, Types of Inorganic Polymerization, Comparison with

organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, coordination polymers, sulphur-nitrogen, sulphur-nitrogen-fluorine compounds, - binary and multi-component systems, haemolytic inorganic systems.

Books Recommended

1. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 6th Edn. (1999), John-Wiley & Sons, New York.
2. James E. Huheey, *Inorganic Chemistry*, 4th Edn. (1993), Addison Wesley Pub. Co., New York
3. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn. (1997), Butterworth Heinemann, London.

CHM 404 (I): Special Topics in Inorganic Chemistry

Credits: 2

1. **Macrocyclic Complexes:** Design and synthesis by coordination template effect, Applications of macrocyclic complexes.
2. **Supramolecular Chemistry:** Concept of supramolecular chemistry, nomenclature, molecular recognition, metallo-macrocycles as receptors: Applications in transport processes.
3. **Molecular Magnetic Materials:** types of magnetic interactions, inorganic and organic ferro-magnetic materials, low-spin–high-spin transitions, molecular magnets and applications.
4. **Metallomesogens:** Basic concepts, synthetic strategies, characterization and applications.

Books Recommended

1. Jean-Marie Lehn, *Supramolecular Chemistry*, VCH, Weinheim (1995).
2. J. L. Serrano, *Metallomesogens*, VCH, Weinheim (1996).
3. Oliver Kahn, *Molecular Magnetism*, VCH, Weinheim (1993).
4. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn., John Wiley & Sons (Asia), Singapore (2003).

Organic Chemistry Specialization

CHM 402 (O): Application of Spectroscopy to Structural Analysis

Credits: 2

1. **PMR Spectroscopy:** Interpretation of spectra, chemical shift, shielding mechanism and anisotropic effects, chemical exchange and chemical shifts in chiral molecules. Spin-spin, spin-lattice relaxations, Spin-spin interactions, naming spin systems, magnitude of coupling constant: Germinal, vicinal and long range couplings. Simplification of Complicated Spectra: Aromatic induced shifts spin decoupling, deuterium exchange, spectra at higher fields. Hindered rotation and rate processes. Nuclear Overhauser effect.
2. **CMR Spectroscopy:** General considerations, chemical shift, calculation of approximate chemical shift values, coupling constants. Interpretation of simple CMR spectra. DEPT spectrum. 2 DNMR: COSY, NOESY and HETCOR.
3. **Mass Spectrometry :** Introduction, ion production, fragmentation, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra
4. **Problems:** Structure elucidation based on spectroscopic data (IR, UV, NMR and Mass).

Book Recommended

- J. R. Dyer, *Application of Absorption Spectroscopy of Organic Compounds*, Prentice Hall, New Delhi (1978).
- R.M. Silverstein and F.X. Webster, *Spectroscopic Identification of Organic Compounds*, 6th Edition (2003) John Wiley, New York.
- D.H. Williams and I.F. Fleming, *Spectroscopic Methods in Organic Chemistry*, 4th Edition (1988), Tata-McGraw Hill, New Delhi.
- P.Y Bruce, *Organic Chemistry*, 2nd Edition (1998) Prentice – Hall, New Delhi.

CHM 403 (O): Reagents and Organic Synthesis**Credits: 2**

- 1. Oxidation :** (i) Oxidation with peracids: Oxidation of carbon-carbon double bonds carbonyl compounds, allylic carbon-hydrogen bonds, (ii) Oxidation with selenium dioxide and Osmium tetroxide, (iii) Oxidation with lead tetraacetate, mercuric acetate (iv) hypervalent iodine
- 2. Reagents and Reactions :** (i) Gilman's reagent – Lithium dimethylcuprate, (ii) Lithium diisopropylamide (LDA), (iii) Dicyclohexyl carbodiimide (DDC), (iv) 1,3-Dithiane (Umpolung reagent), (v) Peterson's synthesis, (vi) Bakers yeast, (vii) DDQ, (viii) Palladium catalysed reactions, (ix) Woodward and Prevost hydroxylation, (x) Iodotrimethyl silane and (xi) Ionic liquids

Books Recommended

1. H.O. House, *Modern Synthetic Reactions*, 2nd Edition (1972), Benjamin/Cummings Publishing Company, California.
2. L.F. Fieser and M. Fieser, *Reagents for Organic Synthesis*, Vol. 1-16 (Vol. 1, 1967), Wiley-Interscience, New York.
3. M.B. Smith and J. March, *March's Advanced Organic Chemistry – Reactions, Mechanisms & Structure*, 5th ed. (2001), Wiley-Interscience, New York.
4. M. B. Smith, *Organic Synthesis*, McGraw Hill Inc., New York (1995).
5. J. Clayden, N. Greeves, S. Warren, and E. Wothers, *Organic Chemistry*, Oxford Univ. Press, Oxford (2001).
6. P. R. Jenkins, *Organometallic Reagents in Synthesis*, Oxford science Publ., Oxford (1992).

CHM 404 (O): Heterocycles**Credits:2**

1. General Considerations: Structure, synthesis and reactivity.
2. Synthesis and reactions of the following ring systems:
 - a. Three-membered rings: Aziridines.
 - b. Four-membered rings: Azetidines and their 2-oxo derivatives.
 - c. Five-membered rings containing two heteroatoms: Oxzoles, Imidazoles, Thiazoles, Isoxazoles, Pyrazoles.
 - d. Pyrimidines.
 - e. Purines: Uric acid and Caffeine.
 - f. Five-membered ring heterocycles with three or four heteroatoms.

Books Recommended

1. T.L. Gilchrist, *Heterocyclic Chemistry*, 3rd Edition (1997) Addison-Wesley Longman Ltd., England
2. R.K. Bansal, *Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms*, 3rd Edition (1999), New Age International, Publisher, New Delhi.
3. A.R. Katritzky, C.A. Ramsden, J.A. Joule and V.V. Zhdankin, *Handbook of Heterocyclic Chemistry*, 3rd Edition (2010), Elsevier, Oxford, UK.
4. *Heterocyclic Chemistry*, 4th ed. J.A. joule and K. Mills Blackwell Publishing, Indian Reprint 2004.
5. *Heterocyclic Chemistry Vol-III,III*, 1st ed. R.R. Gupta, M. Kumar, V. Gupta Springer-Verlag, Berlin Heidelberg Publication(2005)
6. *Aromatic Heterocyclic Chemistry: David T. Davies*, 1992, Oxford University Press.

*Physical Chemistry Specialization***CHM 402 (P): Statistical Mechanics****Credits: 2**

- 1. Basic statistical mechanics:** Phase space, equal a priori probability, ensemble (canonical, micro-canonical and grand canonical), Liouville theorem, entropy, Gibbs paradox.
- 2. Partition function:** Rotational, vibrational, translational, electronic and nuclear partition functions, application of partition functions to specific heat of solids and chemical equilibrium.
- 3. Bose-Einstein and Fermi-Dirac distributions:** Einstein condensation, thermodynamic properties of ideal BE gas, degenerate Fermi gas, application of FD statistics to electron gas in metals.
- 4. Fluctuations:** Means square deviation and fluctuations in ensembles, concentration fluctuations in quantum statistics.

Books Recommended

1. Statistical Mechanics(1988), B.K. Agarwal and M. Eisner, Wiley Eastern, New Delhi
2. Statistical Mechanics(2000), D.A. Mcquarrie, California University Science Books
3. Statistical Mechanics(1996), R. K. Patharia, Butterworth, Heinemann, Elsevier
4. Statistical Mechanics (1962), N. Davidson, Mc Graw Hill Book Co. New York

CHM-403 (P): Solid State Chemistry**Credits: 2**

- 1. Solid state reactions:** General principles and experimental procedure of solid state reactions, growth of single crystals: Czochralski, Bridgman and Stockbarger methods.
- 2. X-ray diffraction and crystal Structure:** Generation of X-rays, diffraction of X-rays by crystals, systematically absent reflections, multiplicities, X-ray diffraction experiments: the powder method and single crystal method, scattering of X-rays by atoms and a crystal, the structure factor, its relation to intensity and electron density, the phase problem.
- 3. Phase transitions:** Thermodynamic and Burger's classification of phase transition, Kinetics of phase transition, nucleation and growth.
- 4. Electronic properties and band theory:** Electronic structure of solids- band theory, Refinement of simple band theory- k-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, p-n junctions; superconductors, Meissner effects, basic concepts of BCH theory.
- 5. Magnetic Properties:** Behavior of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis.

Books Recommended

1. Solid State Chemistry and its Applications(1984), A.R. West, John Wiley and Sons, Singapore
2. Introduction to Solids(1977), L.V. Azaroff, Tata McGraw-Hill, New Delhi
3. Solid State Chemistry(1992), L. Smart and E Moore, Chapman & Hall, Madras
4. Principles of Solid State(1993), H. V. Keer, Wiley Eastern

CHM: 404 (P) Chemical Kinetics**Credits: 2**

1. **Transition state theory:** Application of statistical mechanics to transition state theory, comparison of transition state theory with experimental results, thermodynamic treatment of TST, theories of unimolecular reactions - treatments of: Lindmann, Hinshelwood, Rice-Ramsperger- Kassel (RRK), and Rice- Ramsperger-Kassel-Marcus (RRKM).
2. **Reactions in solution:** Reaction between ions, effect of solvent (single & double sphere models), interpretation of frequency factor and entropy of activation, influence of ionic strength, salt effect, reactions involving dipoles, influence of pressure on reaction rates in solution.
3. **Molecular collisions:** Intermolecular potential and centrifugal barrier, impact parameter, collision cross section and rate, energy threshold, opacity function and reaction cross-section.
Experimental probes of reactive collisions: IR chemiluminescence, laser-induced fluorescence.
 Features of potential energy surfaces (PES), enhancement of reaction.
Molecular beams: Stripping and rebound mechanism.
Dynamics with femtosecond laser techniques: Detection of activated complex.

Books Recommended

1. *Reaction Kinetics*(1998), M. J. Pilling and A.P.W, Seakins, Oxford Science Publication, New York
2. *Chemical Kinetics*, 3rd Edition (1967), K.J. Laidler, Harper & Row Publishers, New York.
3. *Kinetics and Mechanism of Chemical Transformation*, 1st Edition (1993), J. Rajaram and J.C. Kuriacose, MacMillan India Ltd., New Delhi.
4. *Modern Liquid Phase Kinetics*(1994), B. G. Cox, Oxford University Press, Oxford
5. *Molecular Reaction Dynamics and Chemical Reactivity*(1987), R. D. Levine and R. B. Bernstein, Oxford University Press, Oxford
6. *Femtochemistry-Ultrafast Dynamics of the Chemical Bond*(1994), A. H. Zewail, vols. I and II, World Scientific, New Jersey, Singapore

CHM405: Projects**Credits : 5**

Elective Papers

Elective-II (Group-B)

CHM406: Environmental Chemistry

Credits:2

1. **Introduction to Environmental Chemistry:** Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen)
2. **Atmosphere:** Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in atmosphere; Chemistry of ozone layer.
3. **Hydrosphere:** Complexation in natural water and waste-water, Micro-organisms in aquatic chemical reactions, Eutrophication, Microbiology mediated redox reactions.
4. **Lithosphere:** Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.
5. **Chemical Toxicology:** Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.
6. **Air Pollution:** Particulates, Aerosols, SO_x, NO_x, CO_x and hydrocarbon, Photochemical smog, Air-quality standards
7. **Water Pollution:** Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation (Pb, As, Hg)

Books Recommended

1. G.W. Vanloon, S.J. Duffer, *Environmental Chemistry - A Global Perspective*, Oxford University Press (2000).
2. F.W. Fifield and W.P.J. Hairens, *Environmental Analytical Chemistry*, 2nd Edition (2000), Black Well Science Ltd.
3. Colin Baird, *Environmental Chemistry*, W.H. Freeman and Company, New York (1995).
4. A.K. De, *Environmental Chemistry*, 4th Edition (2000), New Age International Private Ltd., New Delhi.
5. Peter O. Warner, *Analysis of Air Pollutants*, 1st Edition (1996), John Wiley, New York.
6. S.M. Khopkar, *Environmental Pollution Analysis*, 1st Edition (1993), Wiley Eastern Ltd., New Delhi.
7. S.K. Banerji, *Environmental Chemistry*, 1st Edition (1993), Prentice-Hall of India, New Delhi.

CHM407: Photo Inorganic Chemistry

Credits:2

Photochemistry of Transition Metal Complexes: Photoreactions of complexes of Cr(III) and Co(III), photo-aquation, photo-substitution and photo-racemization Photochemistry of Ru(bpy)₃²⁺ and its application as photocatalyst for photo-splitting of water, photo-oxidation of 2-propanol and photo-reduction of carbon dioxide, cyanide bridged triruthenium(II) bipy complexes as antenna. Photochemistry of diisocyanide bridged diimers of Rh(I). Applications of quenching and sensitization techniques in the identification of reactive state in coordination complexes.
Photochemistry of Transition Metal Carbonyls and Europium complexes.

Books Recommended

1. D. M. Roundhill, *Photochemistry and Photophysics of Metal Complexes*, Plenum Press, New York and London (1994).
2. G. J. Ferraudi, *Elements of Inorganic Photochemistry*, John Wiley & Sons (1988).
3. V. Balzani and V. Carassiti, *Photochemistry of Coordination Compounds*, Academic Press, London (1970).
4. O. Horvath and K.L. Stevenson, *Charge Transfer Photochemistry of Coordination Complexes*, VCH Publishers Inc. (1993)

CHM408**Bio-Organic Chemistry****Credits:2**

1. **Enzymes, co-enzymes and their mechanism of action:**
Enzymes, Classification, Inhibition. Mechanism of action of chymotrypsin, aldolase, alcohol, lysozyme. Cofactors as derived from vitamins, co-enzymes, prosthetic, prosthetic group and apoenzymes. Structure and biological functions of coenzyme-A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FAD, lipoic acid. Mechanisms of reactions catalysed by the above cofactors.
2. **Nucleic Acids:** Retro-synthetic analysis of Nucleic Acids - Nucleotides, Nucleosides, Nucleobases (A,T, G, C and U), Sugars (Ribose and deoxyribose). Assembly of oligo-nucleotide chain: Synthesis of polymer support, Nucleosides and Nucleotides, solid phase synthesis of Oligo-nucleotides (DNA/RNA) through phosphoramidite and phosphorothionate approach. Application of protecting groups (-NH₂ and -OH functions, Base and Acid labile) and their deprotection and purification. Concept of depurination.
3. **Bio-synthesis:** terpenoids - C₅, C₁₀, C₁₅, C₂₀ units; alkaloids - quinine and morpholine.

Books Recommended

1. A.L. Lehninger, *Principles of Biochemistry*, (1992) CBS Publishers, Delhi.
2. D. Voet, J.G. Voet & CW Pratt, *Fundamentals of Biochemistry*, (1999) John Wiley & Sons, New York.
3. H.R. Mahler and E.H. Cordes, *Biological Chemistry*, 2nd Edition, (1971) Harper and Row Pub., New York.
4. T.C. Bruice and S. Bentkovic, *Bioorganic Mechanisms*, Vol. I & II, (1966) W. A. Benjamin, New York.
5. H. Dugas and C. Penney, *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, (1981) Springer- Verlag, New York.
6. C. Walsh, *Enzymatic Reaction Mechanisms* (1979), W.H. Freeman & Co., New York.
7. Oligonucleotides and analogues: A Practical approach (1991) F. Eckstein. IRL Press, Oxford.
8. Methods in Molecular Biology. Vol. 20 (1993), Sudhir Agrawal. Humana Press Totowa, New Jersey.
9. Oligonucleotide Synthesis. A Practical Approach (1984), M. J. Gait. IRL Press, Oxford.
10. I.L. Finar, *Organic Synthesis*, 5th edition. Vol.2 (1975), Longman Press, USA.

CHM409**Physical Methods in Chemistry****Credits:2**

1. **Photoelectron Spectroscopy and Related Techniques:** Principle and applications to studies of molecules and surface. UPES and XPS. Auger electron and X-ray fluorescence spectroscopy (AES and XRF).
2. **Techniques for Studying Surface Structure:** Low energy electron diffraction (LEED). Scanning tunneling and atomic force microscopy (STM and AFM).
3. **Neutron Diffraction:** Principle and applications.
4. **Fluorescence techniques:** Steady-state fluorescence spectroscopy. Time-resolved (Time correlated single photon counting-TCSPC) fluorescence spectroscopy. Introduction to Single molecule fluorescence and fluorescence imaging.

Books Recommended

1. J.M. Hollas, *Modern Spectroscopy*, 4th edition (2004), John Wiley and Sons, Chichester.
2. C.N. Banwell and E.M. Mc Cash, *Fundamentals of Molecular Spectroscopy*, 4th edition (1994), Tata McGraw Hill, New Delhi.
3. E.M. Mc Cash, *Surface Chemistry*, Oxford University Press, Oxford (2001).
4. A.K. Cheetham and P Day, *Solid State Chemistry Techniques*, Oxford Univ. Press, Oxford (1988).
5. Joseph R. Lakowicz, *Fluorescence Spectroscopy*, 2nd edition, Plenum Press, New York. (1999).

**CHM410: Laboratory work for Computer Applications in Chemistry
(Common to all branches)****Credits: 1**

Computer programming based on FORTRAN and Numerical methods as per the details of the paper CHM-401 (Computer Applications in Chemistry). Exposure to available standard application packages like: Chemdraw, generation of graphs, data sheets creation, and tables using Excel Programme.