

Structure of M.Sc. III and IV: Inorganic Chemistry

Course no.	Course name	Credits
Semester III	Compulsory courses	
DC 320	Coordination and Bioinorganic Chemistry-II	5 Credits
DC 321	Inorganic Reaction Mechanism and Photochemistry	5 Credits
DC 322	Organometallic Chemistry and Homogeneous Catalysis	5 Credits
DC 323	Solid state Chemistry and Characterization by Analytical Methods	4 Credits
DC 328	Inorganic Chemistry Practicals I	4 Credits
DC 329	Inorganic Chemistry Practicals II	4 Credits
Semester IV	Compulsory courses	
DC 420	Inorganic Polymers and Heterogenous Catalysis	6 Credits
DC 421	Inorganic Materials	6 Credits
	Optional course	
DC 424	Inorganic Application in Industry and Medicine	4 Credits
	Compulsory course	
DC 428	Project	7credits
	Total	50 credits



Department of Chemistry University of Pune

M. Sc (Inorganic Chemistry) Syllabus under the credit system at Department of Chemistry, University of Pune, Pune 411007 is effective for the academic year 2010.

The M. Sc. course in Chemistry for two years will consist of 100 credits. Each semester will run for 15 weeks. We will have 70 credits for theory and 30 for practicals and project work.

The proposed structure for M. Sc. Semester III-IV (Inorganic Chemistry) is the following:

Semester 3:

- DC-320: Coordination and Bioinorganic Chemistry-II (5 credits & 60 lectures)
- DC-321: Inorganic Reaction Mechanism and Photochemistry (5 credits & 60 lectures)
- DC-322: Organometallic Chemistry & Homogeneous Catalysis (5 credits & 60 lectures)
- DC-323: Solid state Chemistry and Characterization by Analytical Methods (4 credits & 48 lectures)

Semester 4:

- DC-420: Inorganic Polymers and Heterogeneous Catalysis (6 credits & 72 lectures)
- DC-421: Inorganic Materials (6 credits & 72 lectures)
- DC-424: Inorganic Application in Industry and Medicine (4 credits & 48 lectures)
(OPTIONAL)

Practicals

- DC-328: Inorganic Chemistry Practical I (4 credits, ~7.5 weeks)
- DC-329: Inorganic Chemistry Practical II (4 credits, ~7.5 weeks)
- DC-428: Project Work (7 credits, ~13.5 weeks)

DC-320 : Coordination and Bioinorganic Chemistry-II (5 credits and 60 lectures)

Section I

Coordination Chemistry

(30 Lectures)

1. Theoretical and Practical aspects of Magnetism in Coordination Complexes [15]

- i) Determination of state functions of R-S terms of d^2 and p^2 , transition metal ions.
- ii) Derivation of Van Vleck's expression and μ_{S+O} formula, Quantization of orbital contribution in d^1 ion and quenching in cubic crystal field.
- iii) Magnetic moments based on crystal field ground term, Perturbation Theory and its application, Spin orbit coupling operator for magnetic susceptibility and magnetic moment of T terms and A, E terms .
- iv) Anomalous magnetic moments in magnetically dilute and concentrated system in various symmetrical environments of coordination complexes.

2. Electron Paramagnetic Resonance Spectroscopy (EPR) [6]

- i) Theory and Instrumentation of EPR.
- ii) Spin Hamiltonian, Isotropic and anisotropic EPR spectra, Magic Pentagon rule.
- iii) Applications of EPR spectroscopy: 1) Structural determination of Inorganic complexes. 2) Applications metalloproteins, Fe, Cu.

3. Nuclear Quadrupole Resonance (NQR) [4]

- i) Principle selection rule for NQR.
- ii) Factors for splitting of quadrupole energy levels in NQR, Effect of Magnetic Field.
- iii) Application of NQR: Structural information from NQR.

4. Cyclic Voltammetry (CV) [5]

- i) Principle of Cyclic Voltammetry, typical features of CV curve, CV advantages and disadvantages.
- ii) Instrumentation
- iii) Electrolytes
- iv) Application of CV technique a) Inorganic Compounds b) Organic Compounds.

Books:

1. "Magnetism and Transition Metal Complexes", F. E. Mabbs and D. J. Machin (Chapman and Hall) London (1973).
2. "Introduction to Magnetochemistry", A. Earnshaw, Academic Press, (1968).
3. Elements of Magnetochemistry, R. L. Dutta and A. Syamal, Affiliated East/West Press Pvt. Ltd. 2007.
4. "Physical Methods in Chemistry", R. S. Drago (2nd Edition) (1977).
5. "Electrochemistry for Chemists", D. T. Sawyer, A. Sobkowak, J. L. Roberts Jr. 2nd Edition, John Wiley, Inc. New York, 1995).

Section II

Bioinorganic Chemistry

(30 Lectures)

1. Recapitulation of Biological Roles of Metals & Ligands (3L)
 - a) Structural Information
 - b) Metal Activity, Specificity & Selectivity
 - c) Biochemical Evolution of Metals in Biological System
2. Biological Chemistry of Iron (7L)
 - a) Transport of Iron
 - b) Hemoglobin & Myoglobin (including their model compounds)
 - c) Storage & Transport Proteins of Iron viz., Ferritin & Transferrin
 - d) Cytochromes
 - e) Iron-Sulfur Proteins
3. Biochemistry of Cobalt (3L)
 - a) B12 Coenzymes and Model compounds
 - b) Actions of Cobalmins & Cobinamides
 - c) Adenosylcobalmin as a Coenzyme
 - d) Ribonucleotide reductase
 - e) Methylcobalmin as cofactor
4. Biological Chemistry of Copper (7L)
 - a) Type I, II & III
 - b) Blue Copper Proteins (Plastocyanins Azurins & Blue Oxidases)
 - c) Models of Blue Copper Compounds
 - d) Non-blue copper proteins e.g. Tyrosinase, Galactose Oxidase, SOD etc.
5. Biological Chemistry of Molybdenum (3L)
 - a) Antagonism between Cu & Mo
 - b) Mo cofactors
 - c) ESR Spectra features
 - d) Hydroxylase Enzymes
6. Biological Chemistry of Vanadium and Chromium (2L)

- a) Vanadium proteins including bromoperoxidases
- b) Glucose Tolerance Factor
- c) Vanadium Nitrogenase

7. Biological Chemistry of Zinc (5L)

- a) Carboxypeptidase and Carbonic anhydrase enzymes

Books :

1. Bioinorganic Chemistry : A Short Course –Rosette M.Roat-Malone, Wiley Interscience, 2002.
2. Biological Inorganic Chemistry –An Introduction, Robert Crichton, Elsevier Science, 2007
3. The Biological Chemistry of the Elements- The Inorganic Chemistry of Life J.J.R.Frausto da Silva and R.J.P.Williams Clarendon Press, Oxford,1991.

DC- 321: Inorganic Reaction Mechanism and Photochemistry (30 lectures)

Section I

1. Types of Mechanisms: Basic concepts as stability and lability, stability constants; HSAB principle, chelate effect, Macrocyclic effect; Ligand transfer and electron transfer reactions in coordination compounds, Intimate and stoichiometric mechanism of ligand substitution.
2. Substitution in square planar complexes: trans effect, trans series, applications of trans effect.
3. Substitution in octahedral complexes: S_N1 , S_N2 S_N1CB mechanisms, racemization in coordination compounds, steric effects on substitutions.
4. Electron Transfer reactions: Potential energy diagrams as a conceptual tool, Marcus equation, Types of and factors affecting electron transfer reactions.
5. Inner and Outer sphere reactions.

Books:

1. “Comprehensive Coordination Chemistry”, Pergamon G. Wilkinson, R. D. Gillard and J. A. McCleverty, , Vol. 1, pp 281-322, 331- 379, 385-411, 415-458 (Chapt. 7.4) and

463-471, (1987).

2. "Inorganic Chemistry", D. F. Shriver, P. W. Atkins and C. H. Langford, 2nd edn. Oxford, Chapt.15, p.559, (1994).

References:

1. "Inorganic Chemistry – Principles of Structure and Reactivity", J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th edn. Harper Collins College Publ. New York, Chapt.13, p.537-76, (1993).
1. "Mechanism of Inorganic Reactions in Solution – An Introduction", D. Benson, McGraw – Hill Chapt.15, p.465, (1968).
3. "d- and f- block Chemistry", C. J. Jones, p. 78, 85 and 122. Tutorial Chemistry Texts, E. W. Abel (Ed.), Royal Society of Chemistry, Cambridge (2001).
4. "Basic Inorganic Chemistry", F. A. Cotton and G. Wilkinson, Wiley Eastern Ltd., New Delhi p.154, (1990).

Section II

Inorganic Photochemistry and Reaction types

(30 lectures)

1. Photochemical Reactions: Prompt and delayed reactions, Quantum yield, Recapitulation of fluorescence and phosphorescence. Photochemical reactions by irradiating at d-d and charge transfer bands. Transitions in metal-metal bonded systems. Photochemical reactions involving chlorophyll. Kinetics of excited state processes. (8)
2. Other Reaction types: Oxidative addition, Reductive elimination reactions, Methyl migration and CO insertion reactions. (2)
3. Reactions of coordinated ligands:
 - i) Non-chelate forming reactions: Reaction of donor atoms (Halogenation of coordinated N atoms, Alkylation of coordinated S and N atoms, Solvolysis of coordinated phosphorus atoms). Reactions of non-donor atoms (nucleophilic behaviour of the ligand, electrophilic behaviour of the ligand).
 - ii) Chelate ring forming reactions: (reactions predominantly involving thermodynamic template effects, reactions predominantly involving kinetic effects).
 - iii) Chelate modifying reactions

(12)

4. Isomerization reactions of thermal and photochemical types involving four coordinated and six coordinated metal complexes. Bailar and ray Dutta twist. (4)
5. Solid State reactions: Types of solid-state reactions and their kinetics and mechanisms. (4)

Books:

1. Inorganic Chemistry, D.F.Shriver, P.W.Atkins and C.H.Langford, Oxford, 2nd. edn. 1994.
2. An Introduction to Inorganic Chemistry by K.F.Purcell and J.C.Kotz, Saunders 1990, Chapter 14.
3. Comprehensive Coordination Chemistry, Vol.1. G Wilkinson (Ed) Wiley, New York, 1967.
4. Inorganic Chemistry by J.E.Huheey, E.A.Keiter and R.L.Keiter 4th edn. Harper Collins, 1993
5. Mechanisms of Inorganic Reactions, by C.F.Basolo and R.G.Pearson, Wiley, New York, 1967.

DC-322: Organometallic Compounds & Homogeneous Catalysis (5 credits & 60 lectures)

Section I :

Organometallic Chemistry (30 lectures)

1. Introduction, definition and scope of organometallic Chemistry (4)
 - a) valence electron count
 - b) 18 and 16 electron complexes
2. d-block carbonyls : (4)
 - a) coordination modes
 - b) characterization
 - c) synthesis
 - d) reactions
 - e) carbonyl metallates
 - f) ligands related to CO
3. σ -organyls : Synthesis, bonding, Properties and applications of (4)
 - a) alkyls
 - b) aryls
 - c) alkenyls
 - d) acyl
 - e) alkynyls

4. Metal-Carbon multiple bonded compounds : Synthesis, bonding, Properties and applications of (2)

- b) carbenes
- c) carbines

5. Π -complexes (2)

- a) alkenes
- b) d—and polyenes

6. η^n - C_nR_n carbocyclic polyenes : Synthesis, bonding, Properties and applications of (6)

- a) allyls η^3 - C_3R_3
- b) pentadienyls η^5 - C_5R_5
- c) cyclopropenyls η^3 - C_3R_3
- d) cyclobutadienes η^4 - C_4R_4
- e) cyclopentadienyls η^5 - C_5R_5
- f) arenes η^6 - C_6R_6
- g) cycloheptatrienyls η^7 - C_7R_7
- h) cyclooctatetraenes.

7. Metal-Metal Bonds and Transition Metal atom clusters (2)

8. Transition Metal organometallic intermediates in organic synthesis (6)

- a) nucleophiles
- b) electrophiles
- c) migration
- (d) protective reagents

Books:

1. Inorganic Chemistry 3rd edn. D.F.Shriver and P.W.Atkins, Oxford University Press, 1999, Chapter 16.
2. Organotransition Metal Chemistry, Anthony F.Hill, Royal Society of Chemistry, Tutorial Chemistry Text, 2002. Chapters 1 to 7.
3. Organometallics: A concise Introduction, Ch.Elshebroicn and A Salzer, VCH, Chapters 12 to 16.
4. Organotransition Metal Chemistry: Applications to Organic Synthesis, S.G.Davies, Pergamon 1982.

Section –II

Homogeneous Catalysis

(30 lectures)

1. Introduction to Catalysis, basic principles: Interplay of Kinetics and thermodynamics in chemical reactions and the role of catalysts. Definition of activity, selectivity in catalysis; homogeneous vs. heterogeneous catalysis; importance of homogeneous catalysis in the synthesis of high value chemicals.
2. Characteristics of central metal ions and influence of attached ligands on catalytic activity; important properties of ligands, elementary steps: Important reaction types: Oxidative addition and reduction; elimination, insertion (migratory) reactions, β -hydride elimination, nucleophilic attack, catalytic cycle; catalytic intermediates and their identification through spectral techniques (IR, ESR, NMR....).
3. What are the reactions that olefins undergo? Hydrogenation of olefins; Wilkinson's catalyst; catalytic cycle. Asymmetric hydrogenation (Enantio-selective hydrogenation).
4. Other reactions of alkenes: Isomerization, dimerization, oligomerization, hydrocyanation and metathesis reactions: Common reactive intermediates. Examples of Shell higher olefin process, DuPont Adiponitrile process.
5. Carbonylation reaction: methanol to acetic acid process and the catalysts employed in BASF and Monsanto processes. Carbonylation of alkynes and other substrates for making industrially important chemicals.
6. Hydroformylation: Cobalt and Rhodium complexes, the role of phosphine ligands in regio selective formation of linear aldehydes. Markovnikov and anti-Markovnikov addition and mechanisms.
7. Polymerization: Catalytic cycle for alkene polymerization; Metallocene catalysts, structure, special features and advantages of metallocene catalysts; mechanism of polymerization and stereocontrol by metallocene catalysts.
8. Oxidation reactions; Wacker oxidation, metal-catalyzed liquid phase oxidation (cyclohexane, p-xylene); epoxidation of propylene; Oxo complexes as homogeneous oxidation catalysts; mechanism of oxidation reactions.
9. Asymmetric Catalysis: General features of chiral ligands and complexes; Mechanisms and Catalytic cycles in hydrogenation, isomerization, epoxidation and catalytic reactions of C-C bond formation

Books :

1. Homogeneous Catalysis: The Applications and Chemistry of Catalysis by Soluble Transition Metal Complexes, G.W. Parshall and S.D. Ittel, Wiley, New York 1992
2. Applied Homogeneous Catalysis with Organometallic Compounds, Vols. 1 & 2, edited by B. Cornils and W.A. Herrmann, VCH, Weinheim, New York, 1996
3. Homogeneous Catalysis: Mechanisms and Industrial Applications, S. Bhaduri and D. Mukesh, Wiley, New York, 2000
4. Homogeneous Catalysis: Understanding the Art, P.W.N.M. van Leeuwen, Kluwer Academic Publishers, 2003

**DC-323: Solid State Chemistry & Characterization by Analytical Methods
(4 Credits & 48 lectures)**

Section I

Solid State Chemistry

24 lectures

1. The Structure of solids: (4 L)

The types of matter, classification of solids, close packing of atoms; Voids in closest packings; Radius ratio rule, Structure of ionic Crystals; Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry MX₂, spinel structure, perovskite structure.

2. Crystal Defects and non-stoichiometry: (5L)

Classification of Defects: subatomic, atomic and lattice defects in solids; Thermodynamics of vacancy in metals; Thermodynamics of Schottky defects in ionic solids ; Thermodynamics of Frenkel defects in silver halides; Calculation of number of defects and average energy required for defect, Other examples of defect structure; Non-stoichiometry and its classifications.

3. Diffusion in solids: (4L)

Mechanism of Diffusion; Ficks first law and second law of diffusion in solids; Kirkendal effects in solids.

4. Phase Transformations in Solids: (3L)

Gibbs Phase rule; time scale of phase changes; Phase diagram of binary system; types of phase transitions.

5. Solid State reactions and Crystal Growth (4L)

Classification of solid state reactions and their kinetics and mechanisms; thermal decomposition reaction; law governing nucleation; Growth of nuclei; Reaction between two solids; Improving the reactivity of solids; Zone refining method; Crystal growth.

6. Preparative method of solids: (4L)

Introduction, Ceramic method, microwave synthesis, Sol-gel method, Precursor method, Hydrothermal method, Chemical vapour deposition (CVD) Method, Chemical vapour Transport, Choosing a method for solids.

Books:

1. Solid-State Chemistry an Introduction (2nd Edition) – Lasley Smart and Elaine Moore (Chapman & Hall 1996)
2. Solid State Chemistry- D.K.Chakraborty (New Age International Pvt.Ltd.New Delhi, 2000)
3. Introduction to Solids-L.V.Azaroff (tata McGraw Hill Publication Ltd. New York)
4. Principles of the Solid State-H.V.Keer (Wiley Eastern Ltd.New Delhi, 1994)
5. Solid state Chemistry –N.B.Hannay (Prentice Hall, New Jersey, 1967)

Section II**Characterization by Analytical Methods****(24 L)****1. Thermal Analysis:****(8 L)**

- a) Thermogravimetry (TGA): Definition, Types of TGA, Instrumentation, Information from TGA Curve; Factors affecting TGA curves (instrumental as well as characteristics of sample factors); Application of thermogravimetry; Calculation of percent decomposition and composition of compounds; Limitation and Advantages of TGA.
- b) Derivative thermogravimetry(DTG) and its advantages
- c) Differential Thermal Analysis (DTA) : Definition; Theoretical Basis of DTA;Instrumentation for DTA apparatus; Factors affecting the DTA curve; Application of DTA; Advantages and disadvantages of DTA.
- d) Differential Scanning Calorimetry (DSC) : Definition ; Comparison of DTA and DSC techniques; Istrumentation of DSC, Factors affecting DSC curves.

2. X-ray Diffraction:**(7 L)**

- a) X-ray powder diffraction (XRD):
X-ray source, Diffraction of X-rays,X-ray powder diffraction, Instrumentation and use of standards, identification of compounds using powder diffraction.The importance of intensities, Absences due to lattice centring;Determination of unknown cubic crystal structure by $\sin^2\theta$ method; Parameter to be determined from XRD: Qualitative analysis; Quantitative analysis-percent crystallinity, Crystallite size, surface area, unit cell dimension.
- b) Single crystal X-ray diffraction:
Solving single crystal structures; refining a structure, X-ray crystal structures in the literature.

3. X-ray Photoelectron spectroscopy(XPS): (4 L)

Introduction and basic theory; Instrumentation; Sample selection and preparation, Spectral analysis; XPS imaging.

4. X-ray Fluorescence spectroscopy (XRF) (3L)

Introduction and basic theory; Instrumentation, spectral analysis; Analytical information and applications.

5. Electron Microscopy (2)

a) Scanning Probe microscopy : Scanning Tunneling Microscopy(STM); Atomic Force Microscopy(AFM)

b) Electron Microscopy: Scanning Electron Microscopy(SEM); Transmission Electron Microscopy (TEM).

Books :

1. Thermal Analysis-Wendland
2. Instrumental Methods of Analysis-G-Chatwal and S. Anand (Himalaya Publication;1988)
3. Catalysis: Principles & Applications-B.Viswanathan,S.Savasankar and A.V.Ramaswamy (Narosa Publication; 2004). (For XRD part)
4. Solid State Chemistry: An Introduction-Lesley Smart and Elaine Moore (2nd Edition, Chapman and hall, 1996).
5. Crystallography and its applications-L.S.Dent Glasser (Van Nostrand, 1977)
6. Handbook of Applied Solid State Spectroscopy-D.R.Vij (Springer Science, 2006).
7. Optical Properties and Spectroscopy of Nanomaterials-Jin Zhong Zhang (World Science Publication, 2004).
8. Solid Chemistry :techniques-A.K.Cheetham and P.Day (oxford University Press, 1987).
9. Crystal Structure Analysis- M.J.Buerger (John Wiley, 960).
10. Physical Methods for Chemists-R.S.Drago(2nd Edition, Saunders).

Other Books:

11. Element of X-ray Diffraction-B.D.Cullity (1967)
12. The Synthesis and Characterization of Inorganic Compounds-W.L.Jolly (Prentice Hall, 1970).
13. Synthesis and Techniques in Inorganic Chemistry-R.J.Angelias (2nd Edition, Saunders, 1977).
14. Structural Methods in Inorganic Chemistry –E.A.V.Ebsworth,D.W.H.Rankin and S.Cradock (Blackwell Scientific Publication, 1987).

Semester IV

DC-420 Inorganic Polymers and Heterogeneous Catalysis (6 credits & 72 lectures):

Section I

Inorganic Polymers

(36 L)

- a. **Inorganic polymers:** 1. Bridge between small and infinite molecules, Homopolar Inorganic polymers [Polyboranes and Polysilylenes], Heteroboranes
- b. Heteropolar Inorganic polymers [Rings and chains containing nitrogen, Oxyanions and polyoxyanions, Silicones, Biominerals.
- c. **Metal clusters:** Metal-metal bonds, Framework bonding in metal clusters, Synthesis of metal clusters.

Text book

1. I. S. Butler and J. F. Harrod, Inorganic Chemistry – Principles and Applications, The Benjamin/Cummings Publishing Co., Inc., Redwood City, California (USA) (1989) Chapt. 15 to 17, pp 441-503.

References

1. N. H. Ray, Inorganic Polymers, Academic Press (1978).
2. A. F. Wells, Structural Inorganic Chemistry, 5th edn., Oxford (1984).
3. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill valley, California (USA) (1994).

Section II

Heterogeneous Catalysis

(36 Lectures)

1. The Descriptive Chemistry of Heterogeneous Catalysis:

(4 L)

Definition of Catalysis, classification of catalytic systems, classification of solid catalysts, Adsorption of molecules at the solid surfaces, Adsorbed states of molecules on metals, potential-energy curves for adsorption, descriptive chemistry of chemisorption on metals, chemisorption and catalysis by metals-quantitative aspects, catalysis by unsupported and supported bimetals, Adsorption and catalysis on semiconducting oxides, selective oxidation of hydrocarbons. Different types of reactors.

2. Zeolite Compounds and Heterogeneous Catalysis: (10 L)

(a) Introduction to porous materials:

Classification into micro-, meso- and macro porous materials, the origin of pores and its significance, distinction from condensed materials.

(b) Zeolites:

Definition, natural and synthetic zeolite or aluminosilicates, the primary and secondary building blocks, final framework structures, Lowensteins rule, sodalite and other structures, Nomenclature: Atlas of zeolite; structural distinctions, Novel zeolites, examples of small, medium, large and extralarge pore zeolites; general properties and application of molecular sieves.

(c) Characterization of zeolite:

XRD, SEM and other techniques; spectral techniques: FT-IR and solid-state NMR; sorption capacity, surface area by BET method, pore volume and pore structure, the origin of Brönsted and lewis acidity in zeolites, the number and the strength, techniques for the estimation of acidity: adsorption of bases and IR spectra, temperature programmed desorption of bases.

3. Photocatalysis using semiconducting oxides (4 L)

Introduction, definition of photocatalysis, basic principles involved in photocatalysis, mechanism of photocatalysis, application of photocatalysis in various fields such as water remediation, air cleaning, etc.

4. Heterogeneous catalysis by intercalation compounds: (3 L)

General aspects of interstitial compounds of Graphite, structural aspects of graphite intercalation compounds, physical and chemical properties, catalytic reaction.

5. Heterogeneous catalysis by perovskite- related oxides: (4 L)

Solid state properties of perovskite like oxides, Relation of solid state and catalytic properties perovskites.

6. Heterogeneous catalysis by oxides with Scheelite structure : (4 L)

Ideal crystal structure and physical roperties, catalytic oxidation of olefins, mechanism for catalysis by BiMoO₄: Propylene oxidation to acrolein, propylene amino oxidation to acrylonitrile, Role of bismuth in catalysis.

7. Immobilization of transition metal: complex catalysts on Inorganic supports (i.e

Anchored Catalysts)

(3 L)

General aspects of transition metal complexes as homogeneous catalysts (i.e.heterogenizing); Preparation of organometallic catalyst anchored to silica: preparation of metal ligand complex followed by Anchoring, Preparation of metal complex from previously Anchored phosphines.

8. Application of Heterogeneous catalysis:

(4 L)

Food industry, fine chemicals, petroleum industry, petrochemical industry, heavy inorganic chemicals, catalysis in atmospheric pollution (atlist one example of application should be discuss).

Books:

1. Heterogeneous catalysis principles and application, G.C.Bond.
2. Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs and J. C. Jansen (Elseviver Pub. Amsterdam, 2001)
3. Catalysis: Principles and Applications, B.Vishwanathan, S. Sivasankar and A.V.Ramaswamy (Narosa Pub. House, New Delhi, 2004)
4. Advanced material in catalysis, James J. Burton and Robert L.Garten (Academic press, Newyork, 1977)

DC-421: Inorganic Materials**(6 Credit, 72 Lectures)****Section I (36L)****1. Introduction to Nano-Materials**

Definition and types of nano-materials, why are nano-particles are important? size dependent properties, various techniques for making nano-materials, application of nano-materials.

2. Electronics and optical materials

- (a) **Electronic Materials and their application:** Origin of valence and conduction bands in solids, classification of solids into metals, semiconductor and insulator; type of semiconductivity; mobility of charge carriers, temperature dependent conductivity, some examples of semiconducting materials. Application of semiconducting devices; Metal-Metal junction (i.e. Peltier and Seebeck effects), diodes (p-n junctions), transistors (n-p-n junctions), metal-semiconductor junction

(b) Optical materials and their properties: Photonic devices, Photoluminescence, Crystalline Lasers

3. Magnetic Materials

Atomic magnetism and solids, type of magnetic materials, the exchange interactions, hysteresis loops and their classification, calculation of magnetic moment from saturation magnetization, magnetic domains. Examples of magnetic materials: soft and hard ferrites, i.e. structure and magnetic interactions in spinels, garnets, hexagonal ferrites. Application of magnetic materials

4. Superconducting Materials

Definition of superconductivity, Critical temperature (T_c), Critical field, Bardeen – Cooper - Schrieffer (BCS) theory, properties and classification of superconducting compounds, High T_c superconductivity, Examples of superconducting materials: Structure of $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ oxide, Fullerenes, intermetallic superconductors, synthesis of superconductors. Application of superconducting materials.

Section II (36L)

5. Ceramic Materials

Classification of ceramics, dielectric properties and polarization properties of ceramics, piezo-, pyro- and ferro-electric effect of ceramics, sol-gel processing of ceramics. Examples and application of ceramics: oxides, carbides, borides, nitrides.

6. Composite Materials

Definition, glass transition temperature, fibers for reinforced-plastic composite materials (i.e. glass fibers, carbon fibres, and aramid fibers); concretes and asphalt materials. Application of composite materials.

7. Cementitious Materials

Difference between Blended and Non-Portland cements; Non-portland cements; high alumina cements, calcium sulfoaluminate cements, phosphate cements. Chemicals in cement hydration; hydration process, set retarders and accelerators, plasticizers, slip-casting processing. Application of cementitious materials

8. Bio-materials

Definition, Type of bio-materials; dense hydroxyapatite ceramics, bioactive glasses, bioactive glass ceramics and bioactive composites

Books:

1. Introduction to Solids - L. V. Azaroff (Tata McGraw Hill)
2. Materials Science and Engineering – V. Raghavan (2nd Edition 1980)
3. Elements of Materials Science and Engineering – Van Vlack (5th Edition, Wiley 1988)
4. Nature and Properties of Engineering Materials – Z. D. Jastrzebski (John Wiley Sons, 1989)
5. Principles of Materials Science and Engineering – William F. Smith (Wiley, 1991)
6. Insight into Speciality Inorganic Chemicals – David Thompson (The Royal Society of Chemistry, 1995 chapter 13 and 14)

DC-424 : Inorganic Application in Industry & Medicine (4 credits; 48 Lectures) (OPTIONAL)

Section I

Inorganic Application in Industry (24 L)

- a. **Photographic Products Industry:** Introduction; Conventional silver halide based photography; Colour photography; Special applications of photography such as – photochemical reproduction, photolithography, photo conversion, electro photography, etc.
- b. **Dyes and Pigments:** Introduction; Pigments in foods – naturally occurring plant- and animal- pigments; Synthetic food pigments such as Sunset yellow, Allura red, etc.; pigments in plants – raw materials for paints; Physical properties of the pigments in paints; Brief descriptions of the manufacturing process and use of commonly used pigments such as White lead, Zinc oxide, Titanium dioxide, etc.
- c. **Electrochemical Applications:** Introduction; brief discussion on classical electrodeposition of metals; Advancement in the electrochemical industry – modification of electrode surface, brief discussion with respect to preparations and properties of surface modified electrodes such as nafion modified electrodes, pvp modified electrodes, etc.; Applications of surface modified electrodes such as Electrocatalysis, ion selective electrodes, etc.
- d. **Inorganic Chemicals as metallic Corrosion Inhibitors:**
Introduction, Principles of corrosion inhibitors, corrosion as an electrochemical process, Practical aspects of corrosion inhibition, Anion inhibitor properties in neutral electrolytes, some application of corrosion inhibitors (cooling water

circulation-once through and open systems, engine radiation & cooling systems, central heating system, refrigeration plants and high chloride systems, water for steam raising, corrosion inhibitors for paint coating).

e. Green Chemistry :

Introduction, Designing a Green synthesis, Basic Principles of Green Chemistry, Green Chemistry in Day-to-Day life, Green Chemistry in sustainable development.

Books:

1. Handbook of Industrial Chemistry, Vol.1, by K.H.Davis, F.S.Berner, CBS Publishers, Bangalore
2. Comprehensive Coordination Chemistry, Chapter 57,58.
3. Insight into Speciality Inorganic Chemicals-David Thompson (The Royal Society of Chemistry, 1995)-Chapter 15.
4. New Trends in Green Chemistry (2nd Edition)-V.K.Ahluwalia and M.Kidwai (Anamaya Publishers, 2007.

Section II

Inorganic Application in Medicine (24 L)

1. Overview (2 L)

1. Introduction
2. Metal Ions in Disease
Use of chelating agents
Metalloproteins as Drug Targets
Matrix Metalloproteases
3. Modulation of Cellular responses by Metal-Containing Drugs
4. Metal-Based Chemotherapeutic Drugs
5. Metal Complexes as Diagnostic Agents

2. Cisplatin-based Anticancer Agents (5 L)

Introduction
Clinical Properties
Cisplatin vs carboplatin
Iproplatin
Determination of Platinum Drug Levels and Pharmacokinetics
Platinum Chemistry
Mechanism of Action
Structure-Specific Damage-Recognition Proteins
Mechanisms of Resistance to Cisplatin/Carboplatin
Circumvention of Tumor Resistance to Cisplatin
Development of New Platinum Drugs

Dose Intensification of Cisplatin/Carboplatin
Combinations with Other Anticancer Agents : Paclitaxel
Modulation of Platinum Resistance Mechanisms
Dinuclear and Trinuclear Platinum Complexes as Anticancer Agents
Biological Activity of Polynuclear Platinum Complexes. Summary and p53 status of Human Tumors Treatable by BBR3464
Biological Activity and p53 Status
Comparison with Other Clinical Cross-Linking Agents
Structure-Activity Relationships in Polynuclear Platinum Complexes
DNA Binding of Polynuclear Platinum Complexes
Cooperative Effects In the Solution Structures of Site-Specific (Pt,Pt) Interstrand Cross-Links

3. Transition Metal Complexes as Chemical Nucleases (4 L)

Interaction of Metal Complexes with DNA
Reactions of Metal Complexes with DNA
Nuclease activity of $\text{Cu}(\text{phen})_2^+$

4. Biomedical Uses of Lithium (3L)

Chemistry of Lithium
Distribution of Lithium in the body and in Cells
Studies using Lithium isotopes
Biochemistry of Lithium

5. Bismuth in Medicine (3L)

The Chemistry of Bismuth
Properties of the element
Bi(III) Compounds
Bi(V) Compounds
Bismuth in Medicine
Helicobacter Pylori bacterium
Methods for the study of Bi
Bismuth Citrate Complexes
Bismuth Complexes with Biomolecules
Bismuth binding to oxygen-containing molecules
Bismuth Complexes with thiolate ligands
Bismuth(III) complexes with Metallothionine and Transferrin, Enzyme Inhibition

6. Gold Complexes with Anti-arthritic, anti-tumor and Anti-HIV activity (4L)

Introduction
Chrysotherapy,
History of Medicinal Uses

Gold Chemistry

Oxidation states

Gold(I) complexes

Gold(III) Complexes

Oxidation-Reduction Potentials

Gold Biochemistry and Pharmacology

In-vivo metabolism and ligand displacement

Anti-tumor Activity

Anti-HIV activity

7. Vanadium Compounds as Possible Insulin Modifiers

(3L)

Introduction

Characterization of Vanadium's Insulin-mimetic Effects

Sites of Action of Vanadium

Animal Studies and Human Trials

Toxicological Considerations

Improved Tissue Uptake with Metal Chelation

Books :

1. Uses of Inorganic Chemistry in Medicine Ed. Nicholas P.Farrell
2. Metal Complexes as drugs and chemotherapeutic agents
3. Metal Complexes as Enzyme inhibitors A.Y.Louie and Thomas Meade Chem.Rev., 1999, 99, 2711.

Practicals

DC-328: Inorganic Chemistry Practicals I (4 credits, ~7.5 weeks)

DC-329: Inorganic Chemistry Practicals II (4 credits, ~7.5 weeks)

DC-428: Project Work (7 credits , 13.5 weeks)

DC-328 : Classical Inorganic Chemistry Practicals (4 Credits)

A + B = (3 weeks) 12 days

A. Analysis:

1. Alloy [e.g. iron, chromium and nickel from Stainless steel] 2d
2. Ore [e.g. acid-insoluble matter (combined oxides), iron and titanium from Ilmenite] 2d
3. Analysis of Portland cement 2d
4. Pigment [e.g. chromium from Zinc chrome] 1d
5. Pharmaceutical products [e.g. magnesium from tablet of "Milk of magnesia", calcium from calcium-supplementary tablet, iron and zinc from iron- (and zinc)-supplementary capsule] 1d
6. Consumer products [e.g. aluminium from alum] 1d
7. Ion exchange chromatography [separation and estimation of mixture of zinc (II) and magnesium (II)] 1d
8. Purity & Percentage of Metal in Coordination Complexes. 2d

B. Inorganic Practicals (3 weeks) 12 days

Expt No. 1. Photometric Titrations

- a) CuVs EDTA
- b) FeVs EDTA using salicylic acid 2d

Expt No. 2. Photochemistry of ferrioxalate

- a) Preparation
- b) Photochemistry 2d

Expt.No. 3. & 4 Kinetics by conductometry and spectrophotometry 4d

- a) Preparation

- b) Conductometry
- c) Spectrophotometry

Expt No. 5. To study metal-DNA interaction spectrophotometrically 2d

Expt No.6. New Experiment related to Organometallic Chemistry or Homogenous Catalysis 2d

Each experiment includes standardization of the reagents, calibration of the instrument with known reagents and analysis of an unknown

DC-329 : Instrumental Inorganic Chemistry Practicals (4 Credits)

A . Synthesis and Structural characterization of coordination compounds. (12 days)

- 1) Synthesis of coordination compounds: 2d
 - i) $M(\text{acac})_2 \cdot x\text{H}_2\text{O}$ [where $M^{+2} = \text{Mn}^{+2}, \text{Co}^{+2}, \text{Cu}^{+2}$, $x = 2, 2, 0$ respectively]
 $M(\text{acac})_3$ [where $M^{+3} = \text{Mn}^{+3}, \text{Fe}^{+3}$]
 - ii) $\text{trans}-[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$ / $\text{cis}-[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$
 - iii) $[\text{Ni}(\text{en})_3]\text{S}_2\text{O}_3$ / $\text{Hg} [\text{Co}(\text{SCN})_4]$
 - iv) $[\text{Fe} (1, 2, 4\text{-triazole})_3] (\text{ClO}_4)_2$
 - v) $\text{Fe} (\text{DTC})_3$
2. To determine paramagnetic susceptibility and magnetic moment of coordination compounds by Faraday method. (2d)
3. To determine paramagnetic susceptibility and magnetic moment of coordination compounds by Evan's ^1H nmr method. (2d)
4. To interpret IR spectra of acetylacetonone and it's complex. (2d)
 - i) To determine force constant of >C=O bond.
 - ii) To determine bond lengths of >C=O bond.
 - iv) To identify coordination site & type of coordination.

5. To interpret ESR spectrum of $Mn^{+2}(Oh) / Co^{+2}(Oh) / Cu^{+2}(D_{4h})$ etc. (1d)
To calculate magnetic parameters isotropic, anisotropic viz. g-factor, hyperfine coupling constant etc.
6. To interpret electronic spectra of coordination compounds.
 - i) To determine interelectronic repulsion parameter ($B\text{ cm}^{-1}$) & crystal field parameter ($10 Dq$) using numerical fitting procedure.
 - ii) To calculate bonding parameters β_{35} . (2d)
7. To study cyclic voltammograms $K_3[Fe(CN)_6]$ (1d)

B. Solid State Materials: Preparation, characterization and activity: (12 days)

1. Preparation of solid-state materials: a) NiO b) $ZnFe_2O_4$ or $NiFe_2O_4$ c) Fe_3O_4 d) $BaZrO_3$. (2d)
2. To determine the interplanar spacing and lattice constant and crystallite size by using X-ray diffraction techniques (NiO , Fe_2O_3 and $NiFe_2O_4$). (1d)
3. To determine the band gap of semiconducting materials (NiO / Fe_3O_4) by using direct current electrical conductivity measurement. (2d)
4. To find out the number of water molecules from coordination compounds/ hydrated metal salts by using thermogravimetric technique. (2d)
5. Heterogeneous catalysis.
 - (i) Photocatalytic degradation of dye using TiO_2 nanoparticles (2d)
 - a) time dependent
 - b) catalyst concentration
6. To determine the corrosion rate of metal strips (mild-steel / aluminium) in different conc. of acidic/ alkali medium. (2d)
8. To study the effect of 1, 10 phenanthroline on corrosion inhibition of mild-steel in H_2SO_4 . (1d)

Each experiment includes standardization of the reagents, calibration of the instrument with known reagents and analysis of an unknown

DC-428: Project Work (7 credits , 13.5 weeks)

Syllabus of Organic Part II

Course no.	Course name	Credits
Semester III	Compulsory courses	
DC 330	Advanced Organic Reaction Mechanism and Heterocyclic Chemistry	4 Credits
DC 331	Spectroscopic Methods in Structure Determination	5 Credits
DC 332	Advanced Stereochemistry	5 Credits
DC 333	Pericyclic Reactions, photochemistry and Free Radical Chemistry	5 Credits
DC 338	Mixture Separation	4 Credits
DC 339	Advanced Preparations	4 Credits
Semester IV	Compulsory courses	
DC 430	Synthetic Organic Chemistry	6 Credits
DC 431	Chemistry of Natural products	6 Credits
DC 434	Biogenesis of Organic Compounds (Sectional option)	4 Credits
DC 438	Research Project	7 credits

Syllabus of Organic Chemistry: II

Semester III: 4 courses 19 credits + Practicals course 8 credits =27 credits.

DC-330: Advanced Organic Reaction Mechanism and Heterocyclic Chemistry 4 credits

Carbanions in organic Chemistry (18)

Ionization of carbon hydrogen bond and prototopy, Base and acid catalysed halogenation of ketones, keto-enol equilibria, structure and rate in enolisation, concerted and carbanion mechanism for tautomerism, carbanion character in phenoxide and pyrrolyl anions, geometry of carbanions, hydrolysis of haloforms, Aldol, Mannich, Cannizzaro, Darzens, Dieckmann, Claisen Baylis-Hillman reactions, Knoevenagel, benzoin condensation, alkylation of enolates and stereochemistry thereof, Conjugate additions.(15) Enamines and imine anions in organic synthesis etc.(03)

Neighboring Group Participation (8)

Concept of neighboring group participation (anchimeric assistance) with mechanism, neighboring group participation by π & σ bonds, classical and non classical carbocations, Intramolecular displacement by hydrogen, Oxygen, nitrogen, sulphur and halogen. Alkyl, cycloalkyl, Aryl participation, participation in bicyclic system, migratory aptitude, intimate and solvent separated ion-pair, transannular, pinacole and carbocation rearrangements and related rearrangements in neighboring group participation, NGP in elimination and addition.

Heterocyclic chemistry (22)

Furan, pyrrole, thiophene, benzofuran, indole, benzothiophene, pyridine, quinoline, isoquinoline, imidazole, oxazole, thiazole, purines, pyrimidines
Synthesis of chloroquine, papavarine, amlodipine, bromouidine, ranitidine, Vit-B6, tryptophan, thiamine, histidine.

Books:

1. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
2. . Advanced organic chemistry part-A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
3. Advanced organic chemistry by J. March, 6th Ed.
4. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers. Oxford University Press (2001)
5. Modern Heterocyclic chemistry – L. A. Paquette (Benjamin).
6. Heterocyclic chemistry – J. A. Joule and K. Mills 4th edition Blackwell publishing (2007)

DC-331: Spectroscopic Methods in Structure Determination 5 credits

¹H NMR (16)

Recapitulation of basic principle, Fourier Transform technique, Pulse sequence, relaxation processes. Use of Integration in the quantitative determination of isomers, Factors affecting chemical shifts (inductive, resonance and anisotropic effect with examples), chemical shift of different types of protons (alkane, alkene, alkyne and allene), aromatic protons and effect of substituent, different types of spin coupling, first order analysis of spectra, Ramsay mechanism of

spin coupling, roofing effect with example, different spin systems (AB, AM, AX, ABX/AMX spin systems with examples), calculations of line intensities and chemical shifts in AB spin system, factors affecting coupling constants (dihedral angle, Karplus equation-graph, electronegativity, bond order, hybridization, bond angle with examples), non equivalence due to restricted rotations, rate processes. Effect of high field NMR for simplification of spectra, Shift reagents. Spin decoupling and Nuclear Overhauser effect with examples.

¹³C NMR (10)

Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages. Proton Noise Decoupling technique advantages and disadvantages, off-resonance technique, Chemical shifts of solvents, factors affecting chemical shifts, analogy with ¹H NMR, calculations of chemical shift of hydrocarbons, effect of substituents on chemical shifts, different types of carbons (alkene, alkyne and allene), chemical shift of aromatic carbons and effect of substituent. Chemical shifts of carbonyl, nitrile, oxime carbons.

Two dimensional (2D) (08)

NMR techniques, principle and pulse technique, DEPT with 3 different angles, ¹H-¹H COSY, ¹H-¹³C COSY (HETCOR, HMQC), interpretation of 2D spectra and examples.

Mass spectrometry (16)

Theory, instrumentation various methods of ionization (field ionization, FAB, MALDI, californium plasma), different detectors [magnetic analyzer, ion cyclotron analyzer, quadrupole mass filter, time of flight (TOF)]. Importance of HRMS, Rules of fragmentation of different functional groups, factors controlling fragmentation. Fragmentation of different types of compounds like alkanes alkenes, aromatic compounds, carbonyl compounds, nitriles etc.

Problems (10)

based on joint application of UV, IR, ¹H and ¹³C NMR, 2D and Mass (including reaction sequence).

Books:

1. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).
2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed. John Wiley and Sons.
3. Spectroscopic methods in organic chemistry – D. H. Williams and I. Flemming Mc Graw Hill.
4. Absorption spectroscopy of organic molecules – V. M. Parikh
5. Nuclear Magnetic Resonance – Basic Principles- Atta-Ur-Rehman, Springer- Verlag (1986).
6. One and Two dimensional NMR Spectroscopy- - Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998).
8. Organic structural spectroscopy- Joseph B. Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).

9. Organic structures from spectra- Field L. D., Kalman J.R. and Sternhell S. 4th Ed. John Wiley and sons Ltd.

10. NMR spectroscopy of Organic compounds. Jackmann and Sternhell S

DC-332: Advanced Stereochemistry

5 credits

Conformation and reactivity in acyclic compounds

(06)

Meaning of conformation and physical properties, conformational effects on the stability and reactivity

Stereochemistry of six membered rings

(12)

Shape of cyclohexane ring, monosubstituted and disubstituted cyclohexane, physical properties, conformation and chemical reactivity in cyclohexanes, conformational effects in six membered rings containing unsaturation. Six membered heterocyclic ring

The shapes of rings other than six membered rings

(06)

five membered, rings larger than 6-membered medium rings, conformational effects in medium rings, transannular effects, concept of I strain

Fused rings and bridged rings

(14)

Bicyclic and polycyclic, Occurrence, availability, stereochemical restrictions and reactions of norbornyl system

Allenes, spiranes and biphenyls

(06)

Enantiomerism in allenes, alkylidene cycloalkane, spiranes- configurational nomenclature, correlation of axial dissymmetry and centrodissymmetry.

Resolution methods

(04)

Resolution by mechanical separation of crystals, resolution by formation of diastereomers, second order asymmetric transformation, resolution by equilibrium asymmetric transformation, biochemical asymmetric transformation, criteria of optical purity

ORD and CD

(08)

Stereochemistry of natural products, strychnine, podophyllotoxin

(04)

Books:

1. Stereochemistry of carbon compounds - E. L. Eliel

2. Stereochemistry of carbon compounds - E. L. Eliel and S. H. Wilen

3. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)

4. Stereochemistry of organic compounds –Nasipuri

5. Molecules of Nature

6. Organic Chemistry, Cram, Hammond, Hendrickson

DC – 333:Pericyclic Reactions, photochemistry and Free Radical Chemistry **5 credits**

Pericyclic reactions analysis and their applications in synthesis ,
Recapitulation of Molecular Orbitals, their symmetry properties **(2)**

Woodward –Hoffmann’s Conservation of orbital symmetry property rule. **(6)**
Application of Woodward –Hoffmann’s Conservation of orbital symmetry
property rule to the ground state and excited state Electrocyclic reactions, Cycloaddition reactions
Chelotropic reactions, and Sigmatropic reactions

Fukui’s HOMO and LUMO orbitals **(11)**
Application of Fukui’s HOMO and LUMO orbitals analysis to the ground state and excited state
Electrocyclic reactions, Cycloaddition reactions, Chelotropic reactions and Sigmatropic reactions

Synthesis of Endiandric acid (using pericyclic reactions) **(4)**

Synthesis of Citral (using pericyclic reactions) (BASF synthesis) **(1)**

Photochemistry: **(20)**

Principles of photochemical reactions; orbital symmetry considerations, Excited states and their
properties; experimental set up for photochemical reactions; Several useful photochemical
reactions-olefin, carbonyl, aromatic photochemical reactions and their applications in organic
synthesis (isomerization, Paterno-Buchi reaction, Barton reaction, Norrish type I and II reaction,
Photoreduction, Rearrangements: di- π -methane, oxa di- π - and aza di- π -methane rearrangements,
Photocycloaddition, Photochemical aromatic substitution reaction, Reactions with singlet oxygen.
Applications of photochemical methods in synthesis: Isocumene, Cedrene, Hirsutene.

Free radicals in organic synthesis **(16)**

Formation, stability and detection of long and short lived radicals, homolysis and free radical
displacements, addition and rearrangement of free radicals, radical cyclizations and their
applications in synthesis

Books/References:

1. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
2. Advanced Organic Chemistry, Part A – F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007).
3. Radicals in Organic Synthesis B. Giese, Pergamon press (1986)
4. a) Organic photochemistry: A visual approach-Jan Kopecky, VCH publishers (1992).
b) Excited states in Organic Chemistry- J.A. Barltrop and J.D.Coyle, John Wiley & sons
c) Organic Photochemistry-O. Kan
5. Conservation of orbital symmetry – R. B. Woodward and R. Hoffmann; Verlag chemie, weinheim (1970).
6. Orbital Symmetry : A problem solving approach- R. E. Lehr and A. P. Marchand; Academic (1972).
7. Organic reactions and orbital symmetry, 2nd Ed. T. L. Gilchrist and R. C. Storr; Cambridge University Press.

8. Classics in total synthesis- K. C. Nicolaou and E. J. Sorensen; VHC (1996)
 9. P. A. Wender and J. J. Howbert **J. Am. Chem. Soc.** **103**, 688-690 (1981)
 10. Henning Hopf et al **Eur. J. Org. Chem.**, 567-581, (2005)
 and references cited therein.
 11 Mehta, G.; Reddy, A. V. J. Chem. Soc., Chem. Commun. 1981, 456-457. and references cited therein

DC: 338 Mixture Separation **4 credits**
DC: 339 Advanced Preparation **4 credits**

Semester IV 3 Courses **19 credits** + 1 course inter sectional option **4 credits= 23 credits**

DC – 430: Synthetic Organic Chemistry **6 credits**

(i) Transitional metals complexes in organic synthesis and Boron, Si, Sn Chemistry

Transition metal complexes in organic synthesis-Introduction-oxidation states of transition metals, 16-18 rule, dissociation, association, insertion, oxidative addition, reductive elimination of transition metal **(1)**

Organopalladium in organic synthesis- Heck arylation, allylic activation, carbonylation, wacker oxidation, isomerization formation N-aryl and N-alkyl bond transmetalation, allyl deprotection in peptides, coupling reactions: Stille coupling, Sonogashira and Suzuki coupling reactions and their importance **(6)**

Organo nickels- coupling carboxylation, amination, carbonylation **(1)**

Chromium carbonyls regioselective alkylation and acylation of aromatics, nucleophilic substitution, lithiation reaction **(2)**

Reactions Iron carbonyls, ferrocenes, Fe-cyclopentadiene complex, protection of dienes, isomerization **(2)**

Manganese and Co-carbonyls in hydroformylation, carboxylations, synthesis of silane complexes and their applications Pausal-khand reactions and its applications protection of alkynes by Co_2CO_8 **(2)**

Wilkinson, Noyori, Knowls catalyst of Ruthenium and Rhodium – synthesis and uses its use in hydrogenation reactions-deallylation, C-C, C-O, C-N bond cleavages **(1)**

Organoboranes- preparation and properties of organoborane reagents e.g. RBH_2 , R_2BH , R_3B , 9-BBN, catechol borane. Thexyl borane, cyclohexyl borane, ICPBH_2 , IPC_2BH , Hydroboration-mechanism, stereo and regioselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes. Synthesis of EE, EZ, ZZ dienes and alkyenes. Mechanism of addition of IPC_2BH . Allyl boranes- synthesis, mechanism and uses **(6)**

Synthesis and uses of organo silane and organo tin compounds **(1)**

Olefin metathesis by I^{st} , and II^{nd} generation catalyst, reaction mechanism and application in the synthesis of homo and heterocyclic compounds **(2)**

Development synthesis, structure, application of Organocatalyst **(4)**

(ii) Designing Organic Synthesis, Synthons and Chirons **(16)**

Chiron-definition, types, application of Chiron- use of carbohydrates, alpha-amino acid, alpha-hydroxy acids and terpenes in selected natural product

(iii) Umpolung in organic synthesis **(04)**

(iv) Protection and deprotection for functional groups as hydroxyl, amino, carboxyl and carbonyl

(04)

(v) Aromaticity

Criteria of Aromaticity- **(2)**

(1) The Energy Criterion (2) Structural Criteria, (3) Electronic Criteria, Relationship among the Energetic, Structural, and Electronic Criteria of Aromaticity, Inscribed polygon method for monocyclic compounds

The Annulenes-Cyclobutadiene, Benzene, Cyclooctatetraene, **(4)**
[10]Annulenes, [12], [14], and [16] Annulenes, [18] Annulene and Larger Annulenes,

Other Related Structures-Kekulene, Fullerene, Aromaticity in Charged **(3)**
Rings, Heteroaromatic Systems, Fused-Ring Systems, compounds with exocyclic double bonds, substituted aromatics

Other aromatic compounds-Mesoionic Compounds, **(1)**
The Dianion of Squaric Acid, 1 Mobius aromaticity, Homoaromaticity

(vi) Fragmentation Reactions **(04)**

(vii) Green Chemistry, Supramolecular Chemistry (Crown ethers, Cyclodextrins, entrainers, Calixarenes) and multicomponent reactions **(06)**

Books/References:

1. Modern synthetic reactions – H. O. House (Benjamin)
2. Organic chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
3. Designing of organic synthesis – S. Warren (Wiley)
4. Some modern methods of organic synthesis – W. Carruthers (Cambridge)
5. Organic synthesis – M. B. Smith
6. Organometallics in organic synthesis – J. M. Swan and D. C. Black (Chapman and Hall)
7. Advanced organic chemistry, Part B – F. A Carey and R. J. Sundberg 5th edition (2007)
8. Palladium in Organic Synthesis Richard Heck
9. Organonickel compounds, Jolly
10. Comprehensive organometallic chemistry-Vol. 1-8
11. Chiron approach in organic synthesis – S. Hanessian (Relavent chapters For Chirons)
12. Aromaticity , P. Garratt
13. Carbocyclic non-benzenoid aromatic compounds, D. Lloyd

DC-431: Chemistry of Natural products**6 credits**

Assymmetric synthesis

(24)

Recapitulation of Stereochemical concepts- enantiomers, diastereomers, homotopic and heterotopic ligands, stereoselective and stereospecific reactions, prochirality, Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer, Asymmetric inductions; Chiral pools, Chiral auxiliaries, chiral reagents and catalysts, and templates;

Asymmetric oxidations: Sharpless asymmetric epoxidation, dihydroxylation, aminohydroxylation, Asymmetric reduction reactions: Reduction of ketones, imines and olefins (use of BINOLS)

Asymmetric C-C bond forming reaction: Simmon-Smith reaction, aldol reaction and alkylation based on Evans method, Mukayama aldol reaction, Shibasaki bi-metallic catalyst system; RAMP-SAMP based alkylation strategy, Meyers oxazoline and bis-lactam based methods; Michael reaction, Henry reaction

(Nitro aldol), Baylis-Hillman-Morita reactions, Asymmetric allylation, Asymmetric cycloaddition reactions, Asymmetric hydroformylation.

Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram's rule, Felkin Anh rule, Houk model, Cram's chelate model. Asymmetric synthesis use of chiral auxiliaries, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation. Self regeneration of stereocentre

Advanced Carbohydrate Chemistry

Introduction of sugars, structures of triose, tetrose, pentose, hexose. Fisher projection, D- and L-configuration, Conversion of Fisher projection to furanose and pyranose form, Haworth Structure, 4C_1 and 1C_4 Conformations, anomeric effect, Reactions of five and six carbon sugars, glycoside formation, acetonide formation, reduction, synthesis of D-glyceraldehyde, Killani-Fischer Synthesis, glucal formation and reactions, Ferrier and Hanesian Reaction, Ferrier rearrangement.

(06)

Utilisation of the basic concepts of carbohydrate chemistry in the synthesis of (S) Propanediol, (R) and (S) – Epichlorohydrin, L (+)-Alanine, 11-Oxaprostaglandin F₂ (-) Multistratin, (-) Pentenomycin, (-) Shikimic acid, Carbonolide B. (06)

Synthesis of biologically active Natural products: (12)
Strychnine (Overmann Syn.), Fredrikamycin A(Norman and Coxan), Cephalosporin (Woodward), Estrone, Mifepristone (Vollard), Taxol

Structure determination of Natural products: (10)
Arteannuin B, Hardwickiic acid, and Ajmaline

Organic Chemistry of Drug Design

Organic chemistry of drug design and drug action-quantitative structure activity relationship Hammett equation, Taft equation Hammett analysis-derivations and application in drug design, illustration with examples (4)

Lipophilicity effect measurement of lipophilicities identification of active part molecular graphics and lead modifications (2)

SAR by mass and NMR (1)

Combinatorial chemistry- general aspects, split synthesis, peptide and non peptide libraries (2)

Drug receptor interactions enzyme inhibitor and drug target (3)

Stereoselectivity and drug action, stereoselective synthesis of Ibuprofen, crixivan, propranolol (2)

Books:

1. Asymmetric Reactions and Processes in Chemistry: Ernest L. Eliel
2. Catalytic Asymmetric Synthesis: 2nd Ed., Iwao Ojima
3. Asymmetric Organocatalysis: From Biomimetic Concept to Applications in Asymmetric Synthesis: David MacMillan
4. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)
5. Asymmetric synthesis Vol.1-5 by J. D. Morrison
6. Chirotechnology: Industrial synthesis of optically active compounds, R. A. Sheldon
7. Organic Chemistry - R. P. Morrison and R. N. Boyd
8. Organic Chemistry – I. L. Finar, volume II
9. Chiron approach in organic synthesis – S. Hanessian
10. An introduction to medicinal chemistry- Graham L. Patric Oxford press
11. The organic chemistry of drug design and drug action- R.B. Silverman
12. Exploring OSAR fundamentals and applications in chemistry and biology-Corwin Hansch and Albert Leo

DC-434 Biogenesis of Organic Compounds (Sectional option)**4 credits**

Biogenesis of terpenes: sesquiterpenes, triterpenes and cholesterol,
alkaloids : polyketide

Biogenesis of terpenes – mono terpenes	(02)
Sesquiterpenes	(06)
Triterpenes	(04)
Steroids	(01)
Biogenesis of Alkaloids-	
ornithine based(pyrrolizidine), Lysine based(quinolizidine and indolizidine),Pyridine based	(01)
Tyrosine and modified tetrahydroisoquinoline based alkaloids	(02)
Phenethylisoquinoline and terpinoid tetrahydroisoquinoline (Amaryllidaceae alkaloids)	(03)
anthranilic acid based	(01)
simple Indole and terpinoid indole, ergot based	(05)
Biogenesis of polyketides – saturate and unsaturated fatty acids	(02)
Arachidonic acid cascades – prostaglandins, Thromboxanes and eicosa acids	(02)
Aromatics derived from polyketides	(01)

Synthesis of amino acids, peptides, nucleotides, nucleosides (08)

Mechanism of biological processes (01)

Peculiarities of enzyme mediated reactions and its comparison with synthetic reactions

Mechanisms involving vit. B1, B2, B6, Biotin, NAD/NADP – NADH/NADPH, Folic acid, Riboflavin (09)

Books

1. Peptides: Synthesis, structure and applications, Bernd Gutte
2. Organic Chemistry, H. Dugas
3. Biochemistry by Zubay Chapter 11.
4. Organic Chemistry Chapter 50– J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)
5. Secondary metabolism by J.Mann
6. Medicinal Natural products by P.M.Dewick

DC- 438

Research Project

7 credits

Structure of M.Sc. III and IV: Physical chemistry

Semester III

Compulsory:

Course no.	Course name	Credits
Semester III	Compulsory courses	
DC 340	Quantum Chemistry	4 Credits
DC 341	Nuclear, radiation and photochemistry	4 Credits
DC 342	Physicochemical Techniques	4 Credits
	Optional courses any one from following three	
DC 344	Topics in theoretical chemistry	4 Credits
DC 345	Polymer chemistry	4 Credits
DC 346	Biophysical chemistry	4 Credits
	Compulsory courses	
DC 348	Practical I: Computer programming	3 Credits
DC 349	Practical : II	7 Credits
Semester IV	Compulsory courses	
DC 440	Molecular Structure and Spectroscopy	4 Credits
DC 441	Solid State Chemistry and Catalysis	4 Credits
DC 442	Surface Chemistry and Electrochemistry	4 Credits
	Optional courses any one from following four	
DC 444	Molecular Modeling and Computational Chemistry	4 Credits
DC 445	Special Topics in Nuclear and Radiation Chemistry	4 Credits
DC 446	Special topics in physical chemistry	4 Credits
DC 447	Recent trends in physical chemistry	4 credits
	Compulsory course	
DC 448	Project	8 credits

DC 340: Quantum Chemistry and Statistical Thermodynamics

1. Recapitulation: Classical Mechanics, Lagrangian and Hamilton formulation, Postulates of Quantum mechanics, probabilistic interpretation of wave function, hermitian and linear operators, eigenfunctions and eigenvalues, expectation values, Bohr correspondence principle, theorems for hermitian and linear operators (with proofs) etc. (10L)
2. Angular Momentum: Recapitulation, commutative relations, The method of ladder Operators, Spin. (8L)
3. Approximate methods: The variational theorem, treatment of excited states. Applications to quantum chemistry. Time-independent perturbation theory: nondegenerate and degenerate cases, Introduction to time-dependent perturbation theory. Application (16L)
4. Statistical thermodynamics: Molecular energy levels, Boltzmann distribution law, partition functions and ensembles, calculation of translational, rotational and vibrational partition functions, statistical thermodynamics and second law, calculation of different thermodynamic functions such as energy, heat capacity, entropy, free energy, equilibrium constants, application of statistical thermodynamics, principle of equipartition of energy, Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics. (14L)

Text Books:

1. Quantum Chemistry, *I. N. Levine*, Fifth Edition, Prentice Hall, New York(1998)
2. Physical Chemistry, *P. W. Atkins*, Sixth Edition, Oxford University Press, Oxford (1998)
3. Quantum Chemistry, *D. A. McQuarrie*, Viva Books, New Delhi (2003)
4. Physical Chemistry, *G. M. Barrow*, Fifth Edition, Tata McGraw Hill, New Delhi (1994)

DC 341 Nuclear Radiation and photochemistry

Nuclear and Radiation Chemistry

1. Nuclear fission -: The discovery, conformation of nuclear fission, types of fission reaction, mass distribution of fission product, emission of neutron in fission, fissile and fissionable nuclides, theory of nuclear fission, critical energy for fission, products of nuclear fission (4L)
2. Nuclear reactors :- General aspects of reactor design, thermal, fast and intermediate reactors, reactor fuel materials, reactor moderators and reflects, coolants, control materials, shield, regeneration and breeding of fissile matter, types of research reactors. (4L)

3. Nuclear structure:- The liquid drop model, calculation of nuclear binding energies, properties of isobars, missing elements, the nuclear shell model, magic numbers, filling of nucleon shells, the collective and unified models. (4L)
4. Ion beam analysis techniques: Particle induced X-ray emissions- projectile accelerator and target preparation, ionization and X-ray emission detection, analysis and applications. Rutherford back scattering – scattering reaction, surface analysis, depth profiling, channelling effects and applications (4L)
5. Radiation detectors: Scintillators and their properties inorganic and organic, solid state semiconductor detectors-theory, surface barrier, Li drifted and intrinsic detectors (4L)
6. Radiolysis of aqueous solutions : Radiolysis of water, ferric sulphate, ceric sulphate, cupric sulphate solutions , Radiolysis Kinetics: Pulse Radiolysis and competition kinetics, non-homogeneous kinetics, flash photolysis (4L)

Photochemistry

1. Introduction: Laws of photochemistry, interaction of light with matter, theory of photoluminescence, general features of photochemical and photophysical processes (3L)
2. Mechanism of absorption and emission of radiation: Einstein's treatment, selection rules, Life times of excited electronic states of atoms and molecules Types of electronic transitions in organic molecules photochemical pathways, Jablonski diagram, Fluorescence, Phosphorescence (4L)
3. Fluorescence emission, factors affecting fluorescence, viz. structure, solvent, pH, temperature etc. Triplet state and phosphorescence, heavy atom effect (4L)
4. Photophysical kinetics of uni and bimolecular processes, delayed fluorescence mechanisms, kinetics of collisional quenching, Stern-Volmer equation, quenching by added substances charge transfer mechanism, energy transfer mechanism (5L)
5. Photolysis, Laser-general principles, types of lasers: two, three and four level lasers, solid state Ruby and Nd/YAG laser, self phase modulation, single photon counting, experimental techniques, flash photolysis: conventional microsecond flash photolysis, Nanosecond laser flash photolysis, Actinometry (5L)
6. Frontiers of photochemistry Picosecond, Femtosecond flash photolysis, applications: Solar energy conversion and storage, photosynthesis (3L)

References:

1. Essentials of Nuclear Chemistry, H. J. Arnikar, Wiley Eastern Limited, 4th Edition.(1995)
2. Nuclear and Radiochemistry, G. Friedlander, J. W. Kennedy and J. M. Miller, John Wiley (1981)
3. Introduction to Radiation Chemistry, J. W. T. Spinks and R. J. Woods, John Wiley (1990)
4. Introduction to Nuclear Physics and Chemistry, B.G. Harvey, Prentice hall (1963).
5. Sourcebook on Atomic Energy-S. Glasstone, Van Nostrand Company (1967)
6. Radiochemistry and Nuclear methods of analysis-W.D.Ehman and D.E. Vance, John Wiley (1991)
7. Fundamentals of photochemistry by K.K.Rohatgi-Mukherjee
New Age International Publishers Revised Edition (Reprint 2003)
8. Chemistry and light by Paul Suppan, The Royal Society of Chemistry
9. Introduction to Instrumentation Analysis by R.D. Braun Pharma Med Press

DC-342 Physicochemical Techniques**Physicochemical methods**

1. X-ray methods
Generation and properties of X-rays, generation of X-rays, -spectra, X-ray absorption, Concept of absorption edge, application, X-ray absorptive apparatus, radiography and radiotherapy, applications, X rays fluorescence, fundamental principles, instrumentation, wavelength dispersive and energy dispersive, quantitative analysis, X-ray emission, fundamental principles, X ray diffraction, powder diffractometer, applications in material science, electron microprobe, further advanced techniques, Introduction to STEM, SEM (8L)
2. XPS(X-ray photoelectron spectroscopy) : Theory satellite peaks, chemical shift, apparatus, chemical analysis, using ESCA, AES-fundamental principles UPS (6L)
3. Luminescence, chemiluminescence, gas phase, liquid phase chemiluminescence, apparatus, bioluminescence, electrochemiluminescence (4L)
4. Mass spectrometry: Theory, instrumentation-basic components, ionization sources, analyzers, resolution, chemical analysis, advanced techniques-GC/MS, MS/MS introduction (6L)
5. Neutron Activation Analysis : Principle, target, matrix, cross-section, fluxes, saturation activity, excitation function, Different steps involved in NAA, radiochemical and instrumental NAA, prompt radiation and pulse neutron activation analysis, applications (8L)
6. Inductively coupled plasma atomic emission spectroscopy: principle, instrumentation,analysis and applications (6L)

7. Thermal methods of analysis: TGA, DTA, DSC and thermometric titrations – principle, instrumentation, factors affecting TGA curve, applications (6L)
8. Radiometric titrations : Principle , types and instrumentation (4L)

Text Books

1. Introduction to Instrumental Analysis- R. D. Braun, Pharmamed Press, Indian Reprint (2006)
2. Principles of Instrumental Analysis, 5th edition- D.A. Skoog, F.J. Holler, T.A. Nieman, Philadelphia Saunders College Publishing (1988)
3. Principles of activation analysis - P. Kruger , John Wiley (1971)
4. Nuclear analytical chemistry- J. Tolgyessy and S. Verga Vol. 2 , University park press (1972)

(6L)

DC 344: Topics in Theoretical Chemistry

(Sound mathematical background and a good knowledge of quantum chemistry principles and chemical bonding is a prerequisite for this optional course. Any THREE OF THE FOLLOWING TOPICS will be discussed.

1. Hartree Fock Theory
Slater determinants, Postulate of antisymmetry, Slater-Condon rules for matrix elements, Hartree-Fock equations, Koopmans and Brillouin theorem, Roothaan equations, basis sets, computational aspects, UHF method, Pople Nesbet equations (Ref. 1). (16L)
2. Semiempirical Theories
Recapitulation of Huckel method, extended Huckel method, ZDO approximation, CNDO/INDO methods, Molecular Properties, Computational aspects, MINDO, AM1, PM3 methods, comparison of these methods (Ref. 2 and 4). (16L)
3. Density Functional Theory
Introduction, Hohenberg Kohn Theorem, N and V-representability, Levy Functional, Kohn Sham equations, Functional derivatives and local potentials, Thomas Fermi theory, The Kohn-Sham construction, Fractional occupation numbers, Janak's theorem, Slater transition state, Electronegativity, hardness (Ref. 2). (16L)
4. Configuration Interaction
Multi-configuration wave function, full CI matrix, doubly excites CI, illustrations, Natural orbitals, Introduction to MC-SCF methods. Truncated CI and size-consistency (Ref. 1) (16L)

Text Books:

1. Modern Quantum Chemistry, *A. Szabo and N.L. Ostlund*, Dover, New York (1996).
2. Approximate Molecular Orbital Theory, *J.A. Pople and D.L. Beveridge*, McGraw Hill, New York (1971)
3. Density Functional Theory of Atoms and Molecules, *R.G. Parr and W. Yang*, Oxford University Press, Oxford (1989).
4. Molecular Modeling, *A. Leach*, Longman, London (1996).

DC 345: Polymer Chemistry

1. Introduction to Polymer Science: Basic concepts, History of polymers, Classification of polymers as biological – nonbiological, linear branched network, condensation, addition, homo- and hetero- chain, thermoplastic - thermosetting. Chemical and geometrical structure of polymer molecules, Stereo-regular polymers, Optical and geometrical isomerism (5L)
2. Kinetics and Thermodynamics of Polymerization: Kinetics of addition, condensation and radiation induced polymerization. Thermodynamics of polymer solutions, The Flory-Huggins Theory, Flory Krigbaum and modified Flory-Huggins Theory (4L)
3. Copolymerization: Kinetics of copolymerization, Copolymer equation, Monomer reactive ratios, Instantaneous composition of polymer (4L)
4. Properties of Polymers: Crystalline melting point, The glass transition temperature (T_g), States of aggregation, states of phase, Factors influencing T_g. Determination of T_g by dilatometry, calorimetry. Heat distortion temperature. Properties involving large deformations, melt viscosity, tensile strength, stress, strain, crazing, shear banding, solubility and related properties, electrical and related properties (8L)
5. Molecular Weight and Molecular Weight Determination: Molecular weight distribution, Number average and Weight average molecular weight. Methods for determination of molecular weight – Osmometry-membrane osmometry, vapour pressure osmometry, light scattering, viscosity, ultracentrifugation (5L)
6. Polymer Processing: Plastic technology – molding, extrusion. Fibre technology – textile and fabric properties, spinning, Fibre after treatments (5L)
7. Conducting Polymers and Polymer Gels: Structure, properties, characterization and applications (5L)
8. Polymers of Commercial Importance: Polyethylene, Polyacrylics, Polyesters, Nitrile polymers, Polycarbonates, Polyurethanes, Polytetrafluoroethylene (5L)

9. Natural and Synthetic Rubber: Basics of rubber chemistry, Compounding and vulcanization of rubbers. Applications of rubber (4L)
10. Polymer Degradation, Stability and Environmental Issues : Types of degradation, Thermal degradation, Mechanical degradation, Photodegradation, Degradation by high energy radiation. Chemical, hydrolytic and UV stability. Recycling and biodegradation (3L)

References:

1. Polymer Science and Technology by Joel R. Fried Third edition, 2002.
2. Polymer Science, V.R.Gowarikar , N.V.Vishwanathan and Jaydev Sreedhar Reprint edition, 2002.
3. Text book of Polymer Science, Fred W. Billmeyer Jr. Third edition, 2000.
4. Principles of Polymerization, George Odian, Third edition 2002.
5. Handbook on Conducting Polymers – T.A.Skotheim, Ed Marcel Dekker Inc, New York, 1 and2, 1986.

DC – 346 : Biophysical Chemistry

1. Introduction : The cell and its constituents, proteins, nucleic acids, RNA and DNA, enzymes etc., molecular basis of life, human genome and beyond Transcription and Translation (5L)
2. Bioenergetics and Thermodynamics: Molecular interpretation of Energy and Enthalpy, Non-covalent reactions, hydrophobic interactions, Protein and Nucleic Acids. Biochemical Applications of Thermodynamics, Thermodynamics of Metabolism, Role of ATP in biological Systems (hydrolysis of ATP). Biological Reactions, Double Stranded Formation in Nucleic Acids, Ionic Effect on Protein–Nucleic Acid Interactions (8L)
3. Physical Equilibria: Lipid Molecules and Bilayer Phase Transitions in Lipids, Bilayers and Membranes, Biological Membranes, **Membrane Equilibrium**, Transport through cell membrane, Active and Passive Transport, Osmosis and Diffusion, Muscle Contraction, Energy Generation. Nerve Cells, Neuron: Structure and Functions, Nerve Impulse and its Conduction (8L)
4. Electrophoresis: Gel electrophoresis, DNA Sequencing, Double Stranded DNA, DNA, Finger Printing, Conformations of Nucleic Acids, Pulsed-Field Gel Electrophoresis, Protein Molecular Weight, Protein Charge, Macromolecular Interactions. (6L)

5. Kinetics: Basic Concepts, Enzyme kinetics, catalytic antibodies and RNA enzymes- Ribozymes, Michaelis Menten Kinetics, Competition and Inhibition, Monod-Whyman Changeux Mechanism. Photochemistry and Photobiology, Photosynthesis (6L)
6. Spectroscopy of Biomolecules : Spectra of Proteins and Nucleic Acids, Amino acid, Polypeptides, Secondary structure, Rhodopsin :A Chromophoric Protein, Principles of Circular Dichorism and optical rotator dispersion, applications to biomolecules (7L)
7. Macromolecular structure and X-ray diffraction: Chain configuration and conformations of macromolecules, proteins and polypeptides, problems of protein folding, Fundamentals of X-rays, Braggs Law, Determination of molecular structure, calculation of diffracted intensities from atomic co-ordinates (5L)
8. Biopolymers: Basics, Size of biopolymers, Methods of determining particle shape and molecular weight, Interactions with water (3L)

Reference Books:

1. Biophysical Chemistry By Gurtu and Gurtu, Pragati Edition, 2007.
2. Physical Chemistry, Principles and Applications in Biological Sciences By I. Tinico, K. Sauer, J. Wang and J. D. Puglisi, 4th Edition, Pearson Edition, 2007.
3. Biophysical Chemistry By A. Upadhyay, K Upadhyay and N. Nath, Himalaya Publishing House, 2005.
4. Biophysical Chemistry by James P. Allen,
5. Biophysical Chemistry by C. R.Cantor and P.R. Schimmel, WH Freeman & Company, New York, 2004.

DC 348: Physical Chemistry Practical I (3 credits)

Computer Programming and Applications in Computational Chemistry

Part A: Theoretical background of Computer programming (1 credit)

Introduction to hardware and software, binary and decimal numbers, constants and variables, assignment statement, flow chart and their use, IF and GO TO statements, Do loops. Input, output and format statements, Subroutines and function subprograms. Introduction to programming in BASIC/Fortran/C

Part B: The students are expected to write and execute at least six of the following computer programs in BASIC/Fortran/C (1 credit)

1. Linear regression.
2. Quadratic equation.
3. Simultaneous pH titration.

4. Michaelis Menten based enzyme kinetics.
5. Analysis of amino acid sequencing.
6. Analysis of DNA sequences. Complementary sequences, repeat frequencies etc
7. Handling of atomic coordinates files and distance statistics in large molecules.
8. Determination of number of covalent and weak bonds in a given co-ordinate data for protein molecule.

These programs are only indicative. The instructor may choose other programs to illustrate the use of computers in Chemistry.

Part C: Student are expected to use following packages for computational chemistry (1

credit)

1. Standard *ab initio* and molecular mechanics packages of Computational Chemistry for molecular geometry optimization, energy calculation, molecular physical property evaluation viz. Dipole moment, Atomic charges, Electron density, Molecular electrostatic potential. These properties are only indicative. The instructor may choose other properties to illustrate the applications of computers in Chemistry.
2. Visualization of molecular properties

Examination of the Part A will be taken in the form of written test whereas practical examination will be conducted for Parts B and C.

TEXT BOOKS:

1. Computers and Common Sense *R. Hunt and Shelley*, Prentice Hall, New Delhi (1998)
2. Computer Programming in Fortran-90 *V. Rajaraman*, Prentice Hall, New Delhi (1990)
3. Computer and Chemistry: introduction to programming and numerical methods *T. R. Dickson*, Freeman (1968)
4. Computer programs for chemistry *D. F. Detar* W. A. Benjamin Inc, New York Vol. 1-3 (1968-69)

DC -349: Practical Chemistry Course (M.Sc. - Part II, Physical)

1. Determination of kinetics of photolysis of uranyl oxalate.
2. To determine the ionisation constant (pK_a) of an indicator spectrophotometrically.
3. Determination of equilibrium constant for the reaction, $KI + I_2 \rightarrow KI_3$.
4. To determine critical composition and critical temperature for given naphthalene bi-phenyl binary phase system.
5. Determination of composition and stability constant of a complex formed between iron (III) and sulphosalicylic acid by Job's continuous variation method and verification by slope ratio and mole ratio method.

6. Investigation of the solubility of a three component system and hence draw a tie line on a binodal curve.
7. Construct the ternary phase diagram for microemulsion of Tx-100/water/cyclohexane.
8. To determine the critical micellar concentration (CMC) of sodium dodecylsulphate (SDS) using conductivity method.
9. Determination of surface tension of water in presence of surfactant and hence surface excess by capillary rise method/Du-Nouy Ring tensiometer..
10. Determination of diffusion co-efficient and hydrodynamic radius of $K_3Fe(CN)_6$ by cyclic voltammetry (CV).
11. Determination of the dipole moment of polar molecule in a nonpolar solvent by the measurement of refractive index and capacitance.
12. To investigate reaction between H_2O_2 and KI.
13. Determination of order of reaction by iodine clock method.
14. Thermodynamic parameters of an electrochemical cell, temperature dependence of EMF.
15. Surface tension and parachor of liquids by stalagmometer and differential capillary methods.
16. To determine the dose rate of C0-60 source by Fricke dosimetry
17. Use of thiocyanate dosimeter for determining the radiation dose
18. Determination of half life of radioisotopes in a given mixture
19. Determination of molar magnetic susceptibility by Guoy Technique
20. Determination of magnetic susceptibility and no. of unpaired electrons by Faraday technique
21. Determination of Rate constant (Oxidation/reduction of Substituted benzene) by Pulse Radiolysis technique.
22. Determination of activity coefficient of electrolyte/nonelectrolyte by cryoscopy.
23. To study the formation of complex ions by cryoscopy.
24. Determination of isobestic point of a given dye molecule by spectrophotometric method.

Dry experiments

1. Deducing the structure of an organic/inorganic molecule from its NMR and/or mass/and or IR spectra.
2. Analysis of an ESR spectrum of an organic/inorganic radical.
3. Derivation of geometric and spectroscopic and rotation-vibration spectra of linear molecules.
4. Interpretation of electronic spectrum/identifying chromophores and solvent effect studies.

Books

1. Experiments in Physical Chemistry by Carl W. Garland, Joseph W. Nibier and David P. Shoemaker, Mc Graw Hill Publication.
2. Advanced Physico-Chemical Experiments by J. Rose, Sir Isaac Pitman and Sons Ltd.
3. Systematic Experimental Physical Chemistry by S.W. Rajbhoj and T.K. Chondhekar, Anjali Publication.
4. Experimental Physical Chemistry by V.D. Athawale and Parul Mathur, New Age International (P) Ltd. Publishers.

DC 440: Molecular Structure and Spectroscopy

1. Nuclear magnetic Resonance (NMR): (15L)
General Theory: Spin and Magnetism, interaction of nuclear magnetic moment with external magnetic field, classical and quantum mechanical theories, selection rules and transitions line shape, line broadening effects; Spin lattice and spin-spin relaxation: Bloch's equations and solutions (without derivation) and their physical significance;
High resolution NMR spectra concepts of the chemical shift and coupling constants, theory of chemical shift (for closed shell systems), theory of chemical spin-spin coupling constants- AX, A₂, and AB cases: Instrumental and experimental aspects for high resolution NMR: illustrative applications of high resolution ¹H NMR spectra in solutions. Concepts of the rotating frame pulse NMR; Fourier Transfer NMR: Modern NMR spectrometer application of the pulse method for determination of the spin – lattice relaxation times; Outline and illustrative applications of ¹³C NMR of non-metallic solid- line broadening effects- local field , classical magnetic dipole- dipole interactions, chemical shift anisotropy, Quadrupolar nuclei; Wide line NMR– concept of the second moment of its applications; Introduction to the high resolution solid state NMR- illustrative applications: Exchange effects – illustrations.
2. Electron Spin Resonance (ESR): (10L)
Basic Theory, Electron spin and magnetic moment interaction of electron spin with external magnetic field, the resonance condition g-value, line shape and width and intensities, instrumental aspects- (comparison with NMR- spectrometer); ESR Spectra of organic free radicals in solutions hyperfine interaction and hyperfine coupling constants; concepts of spin polarization; spin density, McConnell equation, ESR spectra of inorganic free radicals- anisotropy of g; ESR spectra of molecules in the triplet state – fine structure, illustrations- naphthalene and other triplet state molecules;

Illustrations of ESR – spectra of transition metal ions- Kramers theorem, Jahn-Teller theorem, The spin Hamiltonian, Exchange effects in ESR, illustrations.

3. Nuclear Quadrupole Resonance (NQR): (7L)
Basic Concepts- Nuclear electric quadrupole moments (eq) electric fields gradients (EFG) at the nucleus, asymmetry parameter between (eq) and (EFG), nuclear quadrupole energy levels, selection rules and transitions quadrupole coupling constants (qcc), influence weak magnetic field, influence of external electric fields; Equipment for observation of NQR, interpretation of NQR data- Townes and Daily theory, applications of NQR.

Text Books for magnetic Resonance

NMR

1. High Resolution N.M.R, *E.D. Becker*, Academic Press (1969)
2. Nuclear Magnetic Resonance *E.R. Andrea*, Cambridge University Press (1955)
3. Pulse and Fourier transform N.M.R, *T.C. Farror and E.D. Becker* Academic Press N.Y (1971)

ESR

1. An introduction to Electron Paramagnetic Resonance, *M. Bersohn & J.C. Baird*, W.A. Benjamin, Inc N.Y. (1966)
2. High resolution ESR Spectroscopy *F. Gerson*, (John Wiley & sons– 1970)

NQR

1. Nuclear Quadrupole Resonance in chemistry, *G.K. Semin, T.A. Babushkina & G.G. Yakobson*, John Wiley & sons, (N.Y.)-(1975)

Electric and magnetic properties of molecules Refractive index and electric permittivity

Polarization and Polarizability, Mossotti –Clausius Equation (8L)

The molar refraction, polar compounds, the measurement of permittivity, the Debye Equation, Experimental methods of Dipole moment– determination, interpretation of molecular dipole moment, the limitations and extensions of the simple treatment of molar polarization. Dielectric breakdown, piezoelectricity, ferroelectrics.

Text Books:

1. Electrical and optical aspects of molecular behaviour *M. Davies*, Pergamon Press
2. Lectures on the electrical properties of materials *L. Solymar and D. Walsh* 4th Edition, Oxford Science Publication.

Magnetic Properties (8L)

Diamagnetisation and paramagnetisation theories, experimental determination of susceptibility and molecular magnetic moments, Zeeman splitting, paramagnetisation of multielectron systems. Ferro and antiferro magnetism, magnetic resonance, some applications

Text Books:

1. Introduction to magnetochemistry. *E. L. Earhshaw* , Academic Press
2. Magnetic Susceptibility. *L.M. Mulay*
3. Treatise on Analytical Chemistry, Part I, Vol IV, Interscience , John Wiley, N. Y 1963

DC 441: SOLID STATE CHEMISTRY AND CATALYSIS

Solid State Chemistry

1. Properties of metals and semiconductors: band theory, types of solids, intrinsic and extrinsic semiconductors, p-n junctions, optical properties, photoconductivity of crystals (7L)
2. Imperfections and related phenomenon: Defects in solids: point defects line defects, diffusion in solids- mechanism, elastic and plastic deformations (5L)
3. Crystal growth techniques: General principles, growth from solution, growth from melts, growth from vapour (4L)
4. Imperfections and physical properties crystals: Electrical properties, Optical properties: Colour centers in ionic crystals: types, creation, Magnetic properties , Thermal properties and Mechanical properties. (8L)
5. Solid state reactions: reactions of single solids and their kinetic characteristics, gas - solid, solid -solid, addition and double decomposition reactions, photographic process (6L)

Text Books:

1. Introduction of Solids L.V Azaroff , Tata McGraw Hill
2. Principles of the solid state H. V. Keer, Wiley Eastern (1993)
3. Selected topics in solid state physics Vol. 12, The growth of crystals from liquids – J. C. Brice, North Holland/American Elsevier (1973)
4. Defects and diffusion in solids. S. Mrowec Elsevier publ.(1960)
5. Treatise on solid state chemistry, ED-N.B. Hannay, Plenum press Vol –2 (1975)

Catalysis

1. Fundamentals of adsorption and catalysis: Physical and Chemical adsorption – adsorption isotherms: evaluation, chemisorption on metals and metal oxides. Catalysis: concept of activity, selectivity, poisoning, promotion and deactivation. Types of catalysis: homogeneous, heterogeneous. Heterogeneous catalysis and catalytic kinetics: concept of Langmuir-Hinshelwood (4L)
2. Preparation and Characterization of Catalyst: general methods for preparation of catalysts: precipitation, sol-gel, hydrothermal, impregnation, hydrolysis, vapour deposition. Activation of catalysts: calcinations, reduction. Catalyst characterization: surface area, pore size distribution, particle size determination, XPS, AES, UV-Vis, FT-IR and thermal methods (4L)
3. Nanomaterials and Catalysis: General definition, Nanochemistry basics, distinction between molecules, nanoparticles and bulk materials. Physico-chemical considerations of nanomaterials. Size-dependent properties. (3L)
4. Catalysis in green chemistry and environmental applications: Purification of exhaust gases from different sources: auto-exhaust catalysts (petrol vehicles, diesel vehicles), VOC removal; ozone decomposition; photocatalysis in effluent treatment. (2L)
5. Photo-catalysis: Photoprocesses at metals, oxides and semiconductors: concepts and mechanism. Photocatalysis application in organic pollutant degradation present in water and air. (2L)

Text/Reference books:

1. W. Adamson, Physical Chemistry of Surfaces , Wiley Intersciences, 1990 (5th edition) 1990.
2. Bond, G C, Heterogeneous Catalysis: Principles and Application. Oxford University Press 1987
3. D.K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, Hardcover - Oct 2008 New Age International Publishers)
4. B.C. Gates, Catalytic Chemistry, John Wiley and Sons Inc. (1992).
5. G. Cao, Nanostructures and Nanomaterials - Synthesis, Properties and Applications, World-Scientific, 2004.
6. P.T. Anastas and J.C. Warner, Green Chemistry, theory and practice,

7. Nick Serpone and Ezio Pelizzetti, Photocatalysis: Fundamentals and Applications, Wiley, New York, NY, 1989.

DC – 442: Surface Chemistry and Electrochemistry: (4 Credits, 48 Lectures)

Surface Chemistry: (24 lectures)

1. Adsorption: (4 lectures)
Adsorption definition, Thermodynamics of adsorption, Langmuir adsorption isotherm, Langmuir constant and Gibbs energy of adsorption, Langmuir adsorption with lateral interaction, BET adsorption isotherm, adsorption on heterogeneous surface, The potential theory of Polanyi.
2. Surface Forces: (6 lectures)
Van der Waals Forces macroscopic solids, Microscopic approach, macroscopic calculation-Lifshitz theory, Surface energy and Hamaker constant, Derjaguin approximation, electrostatic double layer, DLVO theory and application.
3. Liquid Surface: (5 lectures)
Microscopic Picture of liquid Surface, Surface Tension, Equation of Young and Laplace (derivation and application), Curve surface, Kelvin Equation, Capillary Condensation, porous solids and Nucleation Theory.
4. Thermodynamics of Interface: (5 lectures)
The Surface excess, Helmholtz/ Gibbs surface energy and definition of surface tension, interfacial enthalpy, Surface tension of pure liquids, Gibbs adsorption isotherm for two component system (derivation expected), Experimental aspects
5. Surfactant Micelles, emulsions: (4 lectures)
Surfactants, spherical micelles, cylinders and bilayers, critical micelle concentration, thermodynamics of micellization (equilibrium and phase separation model, derivations are expected), Structure of surfactants aggregates, biological membranes, microemulsion, inverse microemulsions, formation and stabilization.

Books:

1. Physics and Chemistry of Interface, second edition, Hans-Jurgen Butt, Karlheunz Graf, Micael Kappl, Wiley VCH (2006), ISBN-13 978-3-527-40629-6
2. Physical Chemistry of Surface, A.W. Admson, fifth edition, Wiley Interscience Publiation (1990)
3. Surfactant Science and Technology, second edition, Drew Myers, VCH Publishers (1992)
4. Principles of Colloids and Surface Chemistry, P.C. Hiemenz Marcel and Dekker, N.Y. (1977)

Electrochemistry: (24 Lectures)

1. Introduction and over view of electrochemical processes: (6 lectures)
Electrochemical cell and reactions, Faradic and nonfaradiac processes, electrochemical Experiments and variables in electrochemical cells, Basic electrochemical thermodynamics, free energy and cell EMF, half reaction and

- reduction potentials, formal potentials , reference electrodes , measurements of potential differences, Electrochemical potentials, Fermi level and absolute potentials, liquid junction potential.
2. Ion-ion interactions : (6 lectures)
ideal_solution, deviation from ideality, Activity and activity coefficient, Debye-Huckel Theory , limited and extended law (derivation expected)
 3. Kinetics of Electrode reactions: (8 lectures)
Essentials of electrode reactions, Butler Volmmer Model for electrode kinetics, One step,one electron process through potential energy diagram, standard rate constants and transfer coefficients, equilibrium condition and exchange current, current over potential equation, current-over potential equation, very facile kinetics and reversible behavior, introduction to microscopic theories of charge transfer, Marcus microscopic model , predictions from Marcus theory, Gerischer model based on distribution of energy states , Tunneling and extended charge transfer.
 4. Electrochemical devices : (4 Lectures)
Batteries and Fuel cells

Books:

1. Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)
2. Electrochemical Methods second edition, A.J. Bard and L.R. Faulkner, John Wiley and Son (2001).

DC 444: Molecular Modeling and Computational Chemistry

(Reasonable mathematical background and knowledge of quantum chemistry principles and chemical bonding is a prerequisite for this optional course. ANY THREE of the FOLLOWING TOPICS will be offered.

1. Semiempirical Methods and Molecular Mechanics
Introduction to Molecular Mechanics, MM2, OPLS, AMBER, SHAPE and related force fields, Recapitulation of Huckel theory, EHT, CNDO, INDO, MINDO/3, AM1 and PM3 methods (Ref. 1 and 5) (16L)
2. Molecular dynamics
Simulations, Principles underlying MD methods, Classical and Quantum molecular dynamics, Applications (Ref. 2 and 3) (16L)
3. Case studies in Applied MO Theory
Structure, energetics, charge distributions and spectral data, interpretations in some simple systems, understanding reactivity, visualization of molecular properties (Ref. 4). (16L)
4. Quantitative Structure-Activity Relationships
Electronic and steric effects on organic reactions, topological indices, Hydrophobic parameter, Octanol-water, Partition coefficients, QSAR of Nonspecific Toxicity,

QSAR of Proteins and Enzymes, QSAR in metabolism, Carcinogenesis and antitumor drugs, CNS agents, Microbial QSAR, Design of Bioactive Compounds (Ref. 1).
(16L)

Text books:

1. Molecular Modelling, *A. Leach*, Longman, London (1996).
2. Introduction to Computational Chemistry, *F. Jensen*, John Wiley, New York (1999).
3. Computational Chemistry (Theories and Models), *D. Cramer*, John Wiley, New York (2002).
4. J. B. Foresman and A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc. (1996).
5. Approximate Molecular Orbital Theory, *J. A. Pople and D. L. Beveridge*, McGraw Hill, New York (1971).

DC445 Special topics in nuclear and radiation chemistry

1. Nuclear reactions: Bethe's notation, types of nuclear reactions, conservation in nuclear reactions, compound nucleus theory, experimental evidence, specific nuclear reactions, photonuclear and thermonuclear reactions. (4)
2. Accelerators: Basic components, Cockroft-Walton accelerator, Van de Graaff accelerator, Linear accelerators, cyclotrons, synchrotrons, (3)
3. Radiation hazards and safety ; Natural and manmade sources of radiations, internal and external radiation hazards, safe handling methods, personal dosimetry, reactor safety, the effects of Three miles and Chernobyl accidents, radiation protecting materials. (4)
4. Biological effects of radiations : The interaction of radiations with biological cells, various stages, somatic and genetic effects, maximum permissible dose-ICRP recommendations (4)
5. Hot atom chemistry : Szilard Chalmers process, chemistry of recoil atoms, recoil techniques, models for retention, annealing reactions, annealing mechanisms (3)
6. Applications of radioisotopes in nuclear medicine and pharmaceuticals: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In vivo diagnostic procedures, in vitro diagnostic testing therapeutic use of radiations, Use of radiation for food preservation and sterilization (8L)

7. The origin of chemical elements, cosmology, primordial nucleosynthesis, stellar evolution and stellar nucleosynthesis, solar neutrino problem, Synthesis of Be, B, Li in cosmos (6L)
8. Management of radioactive waste: liquids, solids and gases (4L)
9. Radiolysis of organic systems : Alkanes, aromatic hydrocarbons, alcohols (4L)
10. Radiolysis kinetics : Empirical rate studies, molecular kinetics, non-homogeneous kinetics, effect of solute concentrations on the molecular yields from water, radical scavenging, chain reactions, pulse radiolysis (8)

References

1. Radiation Chemistry: Principles and Applications, Farhataziz and M. A. J. Rodgers (Eds.), VCH Publishers, New York (1987).
2. Radiation Chemistry: Present Status and Future Trends, C. D. Jonah and B. S. M. Rao (Eds.) Elsevier, Amsterdam (2001).
3. Essentials of Nuclear Chemistry: H. J. Arnikar. New Age Publication Ltd. (1995).
4. Radiation chemistry and Nuclear Methods of Analysis W. D. Ehmann, D. E. Vance. John Wiley (1991).
5. Nuclear and Radiochemistry G. Friedelarder, J. W. Kennedy, E. S. Macias, J. M. Miller John Wiley (1981).
6. Source Book of Atomic Energy, S. Glasstone, D. Van Nostrand (1967)

DC-446: Special Topics in Physical Chemistry

Any TWO of the following modules:

A) Chemical Kinetics (2credits) (24L)

Reactions at liquid surfaces- introduction, Cage effect, Friction and diffusion, Langevin Equation, diffusion control, ionic strength and electron transfer, Marcus Theory, Temperature jump and ultrafast laser techniques

Reactions at Solid Surfaces- Adsorption and desorption, Competitive adsorption, catalysis, unimolecular and bimolecular surface reactions, A.C.T of surface reactions, surface diffusion, Temperature Programmed desorption and modulated molecular beam methods

Molecular Reaction Dynamics, collisions, Potential energy surfaces, trajectory and semiclassical calculations. Molecular energy (translational, rotational, vibrational, electronic)

transfer, reactive collisions- orientation, bond-selective Chemistry, Potential energy surfaces from Spectroscopic Information, van der Waals Complexes

B) Thermodynamics (2credits) (24L)

Non-equilibrium thermodynamics: (12L)

Entropy of irreversible processes – Clausius inequality; entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy flow; Entropy production in open systems; Rate of entropy production – generalized forces and fluxes; Phenomenological equations, Onsager reciprocity relation; Electrokinetic phenomena; TPD and Thermomechanical effects; Stationary non-equilibrium states – states of minimum entropy production; non-linear thermodynamics of irreversible processes; Some important applications

Thermodynamics of real gases (12L)

Concept of activity, choice of standard states, Methods of determining activity coefficient and activity coefficient, variation of activity and activity coefficient of a gas with pressure and temperature, activity of solids and liquids, concept of fugacity, variation of fugacity with pressure and temperature, fugacity of solids and liquids, fugacity of a gas in mixture of real gases, determination of fugacity of gas in a mixture

Text book:

C. Kalidas and M. V. Sanganarayana. *Non-Equilibrium Thermodynamics – Principles and Applications*, Macmillan India (2002)

Reference book:

1. Prigogine. *Introduction to Thermodynamics of Irreversible Processes*, Interscience New York (1967) (
2. Katchalsky, A. & Curran, P. F. *Non Equilibrium Thermodynamics in Biophysics* Harvard University Press: Cambridge (1965).

C) Advanced Electrochemistry (2 credits) (24L)

1. Electrical double layer and electrified interface: Thermodynamics of Electrified interface, Electrocapillary curve, Potential of zero charge, structure of electrified interface, parallel plate condenser model: Helmholtz-Perrin Theory, Gouy-Chapman Diffused Charge Model, Potential drop at diffuse layer, Stern model (7L)

2. Electrode: Butler volmmer formulation, Microscopic theories of charge transfer, Marcus microscopic model (derivation expected) , predictions from Marcus theory, Semiconductor electrodes and electron-transfer processes at the semiconductor/electrolyte interfaces, Effect of light at semiconductor-solution interface. (10L)

3. Electrochemical methods: Introduction to Laplace transformations, Boundary condition, Cottrell equation, Controlled Potential Techniques, Electrochemical instrumentations, Scanning probe techniques in electrochemistry. (7L)

Recommended Texts:

1. Bard, A. J. Faulkner, L. R. *Electrochemical Methods: Fundamentals and Applications*, 2nd Ed., John Wiley & Sons: New York, 2002.
2. Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)
3. Antropov, L.I. *Theoretical Electrochemistry*

DC 447: Recent Trends in Physical Chemistry (4 credits; 48 L)

TEM: The Electron Gun, Electron acceleration, Condenser- Lens System, The specimen stage, TEM Imaging System, Vacuum System, Brief outline of TEM Specimens and images (8)

SEM : Operating Principles of the SEM, Penetration of Electrons into a solids, Secondary- Electron images, Backscattered electron Images, SEM operating Conditions, SEM specimen Preparation, The environmental SEM, Electron Beam Lithography (8)

AEM (Analytical Electron Microscopy): The Bohr Model of the atom, X-ray Emission Spectroscopy, X-ray Energy Dispersive Spectroscopy, Quantitative analysis in TEM, Quantitative analysis in SEM (8)

Introduction to Nanoworld, Metals, Semiconductor Nanocrystals, Ceramics, Metal nanoparticles: Double layers, optical properties and Electrochemistry, Magnetism, Chemical and Catalytic aspects of Nanocrystals, Applications of nanoparticles. (12)

4. Title: Introduction to Nanoscale Science and Technology

Edited by: Massimiliano Di Ventra, Stephane Evoy and James R. Heflin, Jr.
Publisher: Springer (Available at NCL Library).

Self assembly and Self Organization: The advantages of Self assembly, Intermolecular Interaction and Molecular Recognition, Self assembly Monolayers (SAMs), Electrostatic Self assembly, Self organization, in Block Copolymer (12)

References

1. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM and AEM by Ray F. Egerton Springer
2. Handbook of Instrumental Techniques for Analytical Chemistry
Editor by Frank Settle Pearson Education (Singapore).
3. Nanoscale Materials in Chemistry
Editor by Kenneth J. Klabunde
John Wiley & Sons

DC 448 : Projects 8 Credits

Syllabus of Analytical Chemistry Part II

Course no.	Course name	Credits
Semester III	Compulsory courses	
DC 350	Principles and Applications of Analytical science	5 Credits
DC 351	Advanced Analytical Techniques	5 Credits
DC 352	Analytical Chemistry of Pharmaceuticals and Polymeric materials	5 Credits
DC 353	Clinical and Consumer Product Analysis	4 Credits
DC 358	Analytical Chemistry Practicals I	4 Credits
DC 359	Analytical Chemistry Practicals II	4 Credits
Semester IV	Compulsory courses	
DC 450	Industrial Products and Forensic Analysis	6 Credits
DC 451	Environmental Chemistry	6 Credits
DC 454	Biomaterials and Agrochemicals	4 Credits
DC 458	Project Work	7 credits

Department of Chemistry
University of Pune

M. Sc (Chemistry) Syllabus under the credit system at Department of Chemistry, University of Pune, Pune 411007 is effective from the academic year 2009.

The M. Sc. course in Chemistry for two years will consist of 100 credits. Each semester will run for 15 weeks. We will have 70 credits for theory and 30 for Practicals and project work.

The proposed structure for M. Sc. Semester III-IV (Analytical Chemistry) is the following:

Semester 3:

DC-350: Principles and Applications of Analytical science (5 credits and 60 lectures)

(Inorganic Section)

DC-351: Advanced Analytical Techniques (5 credits and 60 lectures) (Physical Section)

DC-352: Analytical Chemistry of Pharmaceuticals and Polymeric materials (5 credits and 60 lectures) (Organic Section)

DC-353: Clinical and Consumer Product Analysis (4 credits and 48 lectures) (Biochemistry Section)

Semester 4:

DC-450: Industrial Products and Forensic Analysis (6 credits and 72 lectures) (Inorganic Section)

DC-451: Environmental Chemistry (6 credits and 72 lectures) (Physical Section)

DC-454: Biomaterials and Agrochemicals (4 credits and 48 lectures) (Optional)

Biomaterials – Synthesis and Applications (Biochemistry Section)

Agrochemicals – Synthesis and Applications (Organic Section)

Practicals

DC-358: Analytical Chemistry Practicals I (4 credits, ~7.5 weeks)

Inorganic Analysis (3 / 4 weeks) (Inorganic Section)

Clinical Analysis (3 / 4 weeks) (Biochemistry Section)

DC-359: Analytical Chemistry Practicals II (4 credits, ~7.5 weeks)

Drugs, agrochemicals, etc. (3 / 4 weeks) (Organic Section)

Instrumental Analysis (3 / 4 weeks) (Physical Section)

DC-458: Project Work (7 credits, ~13.5 weeks)

SEMESTER 3

DC – 350: Principles and Applications of Analytical Science (5 Credits) (60 Lectures)

Section I:

(30 Lectures)

a. Analytical Science – a perspective:

History of Analytical Chemistry, Basic concepts, Classical and Instrumental methods, Chemometrics, Automated Analysis, Future trends in Analysis.

b. Sample Dissolution Methods for Elemental Analysis:

Inorganic samples: Introduction, Acids as solvents, Fusion process, and miscellaneous procedures.

Organic samples: Dry and wet ashing methods, Special methods, Dissolution of organic samples.

c. Signal Processing:

(1) Simple D. C. and A. C. Circuits: D. C. Circuits, Current and Potential measuring devices, A. C. Circuits

(2) Electronic Circuits: Semiconductors, Diodes, Transistors, and Practical Circuits and Power Supplies.

(3) Operational Amplifiers and Microprocessors: Integrated Circuits, Op Amp, Logic devices and Computers.

d. Heterogenous Catalysis:

(1) Basic Principles of heterogenous catalysis.

(2) Different types of reactions

(3) Characterization of Heterogenous Catalysis

(4) Photocatalysis

Text Books:

1. "Principles and Practice of Analytical Chemistry", F. W. Fifield and D. Kealey, 5th

- edn., Blackwell Science, Chapt. 1, pp 12-13, 331- 379, 385-411, 415-458 (Chapt. 7.4) and 463-471, (2000).
2. "Fundamentals of Analytical Chemistry", D. A. Skoog and D. M. West, 4th edn., CBS College Publishing, New York, Chapt. 1, pp 12-13, (1982).
 3. "Introduction to Instrumental Analysis", R. D. Brown, McGraw Hill, Chapt. 2,3 and 4, (1987).
 4. "Instrumental Methods of Analysis", H. H. Willard, L. L. Meritt and J. A. Dean, Affiliated East-West Press, Chapt. 1 and 2, (1977).
 5. Heterogenous Catalysis : Principles and Applications by G.C. Bond, Clarendon Press-Oxford, 1974.

References:

1. "Principles of Instrumental Analysis", D. A. Skoog, F. James Hollier and T. A. Naiman, Harcourt College Publishers (1998), Harcourt India Pvt. Ltd., Indian Reprint Chapt. 1, pp 12-13, (2001). / "Principles of Instrumental Analysis", D. A. Skoog, F. James Hollier and S. R. Crouch, 6th edn., Thomson Brooks/Cole Publishers (2007).
2. "Sample Pre-treatment and Separation", R. Anderson, ACOL Series, N.B. Chapman (Ed.), John Wiley & Sons for ACOL, Chapt. 3 and 4, pp 66-118, (1991).

Section II:

(30 Lectures)

- a. Calibration methods
- b. Optimization and Experimental Design
- c. Process Analysis
- d. Quality Assurance and Quality Control
- e. Reference Materials

(3

L)

- a. Calibration : , construction of calibration curves, comparison with single standard, matrix

matching, bracketing of std, standard addition and internal standard methods, calibration of glassware, buoyancy errors, numericals

(5 L)

b. Optimization and Experimental Design : Accuracy, precision, classification of errors, minimization of errors, significant figures and computation, mean deviation and standard deviation, Detection, reduction and compensation of errors, propagation of intermediate error,

confidence level, confidence limit when sigma is known and when sigma is unknown, statistical treatment of random error, properties of Gaussian distribution, Test of significance,

F test, Q test (Student T test), Construction and interpretation of graphs, fitting the least squares lines

(6 L)

c. Process Analysis :Introduction, Hazards, Safety, continuous or regular monitoring, measurement systems, process chromatograph, process sampling and sample systems, service and maintenance, electrochemical methods, ISEs, spectroscopic methods (14 L)

d. Quality Assurance and Quality Control : A) Industrial Analysis : Quality characteristics of chemical analysis, errors occurring at the start, during or by the end of analysis, interpretation

and presentation of results, Shewhart Chart, CUSUM chart and EWMA chart; Batch and process evaluation, QA schemes, experimental designs for optimization studies and ruggedness testing, system management; B) Clinical Analysis : Introduction, analytical responsibilities, Managerial responsibilities, practical approaches to QA, characterization of

a

method, Results and preparation of reports. Internal QC, Accuracy and external quality assessment, near-patient testing and QC; C) Water Industry : Water quality field sampling QA/QC program, QA/QC documentation, QA project plan, designing a water quality monitoring plan, Site selection, sampling frequency and sample size, cost considerations, training of field personnel, field trip preparations, Water quality sampling, toxic chemicals

in

bottom sampling and biota, bacterial sample collection, sequential triplicate sampling, sample

handling, preservation, storage and transport, chain of custody, field safety, field audit program, laboratory QC procedures inter- and intra-laboratory QC, detection limits, reporting of analytical results, data handling and data management

(2 L)

e. Reference Materials (RMs) : Analytical standards, primary and secondary standards, high purity substances, reference materials, use of RMs in statistical control schemes and in intercomparisons, role of certified reference materials (CRMs), production and requirements,

obtaining reference value and certified value

References

1. D. A. Skoog , D. M. West and F.J.Holler, Fundamentals of Analytical Chemistry, 2nd Ed., Saunders College Publishing, 1991.
2. R.A.Day and A.L.Underwood, Quantitative Analysis, 6th Ed., Prentice-Hall of India Pvt.Ltd., 1993.
3. Gas Chromatography, Open Book Learning Series
4. Larry Hargis, Analytical Chemistry. Principles and techniques
4. Encyclopedia of Analytical Chemistry, Vol.

DC-351: Advanced Analytical Techniques (5 Credits) (60 Lectures)

Section –I:

[Total 30 Lectures]

Electrochemical Methods of Analysis:

[10 Lectures]

Polarography: Principles, Factors affecting polarographic wave, pulse polarography, and differential pulse polarograph,

Voltammetry : Voltammetric principles, Hydrodynamic voltammetry, Stripping voltammetry, Cyclic voltammetry, criteria of reversibility of electrochemical reactions, quasi-reversible and irreversible processes, qualitative and quantitative analysis by these techniques. Coulometry and electrogravimetry.

Thermal Methods of Analysis:

[6 Lectures]

Principle and instrumentation of TGA, DTA, DSC & EGA. Thermometric titrations. Typical applications of each technique.

Radiochemical Methods :

[10 Lectures]

Neutron activation analysis : Principle, Definition of various terms, various steps involved.

Absolute & comparative method, PLNAA pulse N

Isotope Dilution analysis : Principle, Direct, reverse double derivative IDA.

Radiometric titration : Principle, types and instrumentation.

Radio immunoarray : principle and applications

Chemically Modified /Ion Selective Electrodes :

[4 Lectures]

Section - II

[Total 30 Lectures]

a. Laser Based Techniques :

[8 Lectures]

Atomic fluorescent spectrometry (AFS), Resonant ionisation spectroscopy (RIS), Laser enhanced ionization (LEI). Principle – types of transition tunable laser, Classification of medium pumping and controlling mechanisms, Instrumentation detailing of various gaseous, liquid and solid sources, cell, monochromators, detectors.

Atomic Emission Spectrometry (AES):

[4 Lectures]

Inductively coupled plasma – ICP / AES and Flame emission spectroscopy (FES). Sources – electrical discharge, dc/ac arcs, spark laser microprobe, qualitative and quantitative analysis, problems discussion

Atomic Absorption Spectrophotometry (AAS):

[6 Lectures]

Principle-spectral line width, doppler and pressure broadening, Instrument-sources-line and continuous, electrodeless discharge lamps, Hollow cathode lamps, temperature gradients, cells – flames, furnaces, detectors, interferences and modifications in instrumentations, applications – problems discussions.

b. Hyphenated techniques:

[4 Lectures]

GC-MS, ICP-MS, tandem mass spectroscopy, MS-MS principle, Instrumentation and analysis of micronutrients like Mo, B, Cu, Zn essential towards the healthy growth of crops, fruits-hence determination of these from soil, plants, fruits etc.

c. Imaging techniques including MRI :

[6 Lectures]

Magnetic resonance imaging (MRI)- principle, instrumentation, magnetic resonance angiography, ^1H nmr of relevant diamagnetic and paramagnetic compounds, contrast agents and clinical applications.

d. Supercritical Fluid Chromatography: [2 Lectures]

Principle, instrumentation and applications in pharmaceuticals.

Books

1. "Introduction to instrumental analysis" R. D. Braun (1987)
2. "MRI : Basic principles and applications", M. A. Brown, R. C. Semelka (1995).
3. "Handbook of Atomic Absorption & Fluorescence Spectrometry by Michael Sargent & Gordon Kirkbright, Viridian Publishing
4. "instrumental methods of chemical analysis", H. H.m Willard, L. L. Merrit Jr., J. A. Dean and F. A. Settle, 6th Edn (1986).
5. Encyclopedia of Analytical Chemistry (1995).
6. "Cyclic Voltammetry and Frontiers of Electrochemistry", N. Noel, and K. I. Vasu, IBH, New Delhi (1990).

DC-352:

**Qualitative and Quantitative analysis of Organic Compounds by spectral methods /
Spectroscopic methods in Structure Determination (5 Credits) (60 Lectures)**

¹H NMR: Recapitulation of basic principle, Fourier Transform technique, Pulse sequence, relaxation processes. Use of Integration in the quantitative determination of isomers, Factors affecting chemical shifts (inductive, resonance and anisotropic effect with examples), chemical shift of different types of protons (alkane, alkene, alkyne and allene), aromatic protons and effect of substituent, different types of spin coupling, first order analysis of spectra, Ramsay mechanism of spin coupling, roofing effect with example, different spin systems (AB, AM, AX, ABX/AMX spin systems with examples), calculations of line intensities and chemical shifts in AB spin system, factors affecting coupling constants (dihedral angle, Karplus equation-graph, electronegativity, bond order, hybridization, bond angle with examples), non equivalence due to restricted rotations, rate processes. Effect of high field NMR for simplification of spectra, Shift reagents. Spin decoupling and Nuclear Overhauser effect with examples.

(16)

¹³C NMR: Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages. Proton Noise Decoupling technique advantages and disadvantages, off-resonance technique, Chemical shifts of solvents, factors affecting chemical shifts, analogy with ¹H NMR, calculations of chemical shift of hydrocarbons, effect of substituents on chemical shifts, different types of carbons (alkene, alkyne and allene), chemical shift of aromatic carbons and effect of substituent. Chemical shifts of carbonyl, nitrile, oxime carbons.

(10)

Two dimensional (2D): NMR techniques, principle and pulse technique, DEPT with 3 different angles, ¹H-¹H COSY, ¹H-¹³C COSY (HETCOR, HMQC), interpretation of 2D spectra and examples.

(08)

Mass spectrometry- theory, instrumentation various methods of ionization (field ionization, FAB, MALDI, californium plasma), different detectors [magnetic analyzer, ion cyclotron analyzer, quadruple mass filter, time of flight (TOF)]. Importance of HRMS, Rules of fragmentation of different functional groups, factors controlling fragmentation. Fragmentation of different types of compounds like alkanes alkenes, aromatic compounds, carbonyl compounds, nitriles etc. (16)

Problems based on joint application of UV, IR, ^1H and ^{13}C NMR, 2D and Mass (including reaction sequence).

(10)

Books:

1. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).
2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed. John Wiley and Sons.
3. Spectroscopic methods in organic chemistry – D. H. Williams and I. Flemming Mc Graw Hill.
4. Absorption spectroscopy of organic molecules – V. M. Parikh
5. Nuclear Magnetic Resonance – Basic Principles- Atta-Ur-Rehman, Springer- Verlag (1986).
6. One and Two dimensional NMR Spectroscopy- - Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998).
8. Organic structural spectroscopy- Joseph B. Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).
9. Organic structures from spectra- Field L. D., Kalman J.R. and Sternhell S. 4th Ed. John Wiley and sons Ltd.
10. NMR spectroscopy of Organic compounds. Jackmann and Sternhell S

DC- 353: Clinical, food and consumer product Analysis (4 Credits) (48 Lectures)

Clinical analysis:

- Enzymatic and Immunochemical Analysis
- Mineral metabolism, Electrolyte analysis
- Body fluid analysis
- Therapeutic drug monitoring
- Scope of Clinical chemistry: Philosophy of clinical analysis, Practical aspects of analysis: sample types, collection of specimens (samples) like blood, urine, faeces; Cleaning of glass apparatus; Storage of clinical samples.
- General techniques for analysis: Brief principle and applications of following techniques: colorimetric, spectrophotometric, turbidimetric, fluorimetric, flame photometry, autoanalysis, paper electrophoresis, gel-electrophoresis, chromatography; Units of expressing biochemical values.
- Protein structure and analysis: Definition of protein and peptides; structure of protein; types of proteins; Physical and chemical properties of protein; Analysis of proteins: Total protein, albumin and globulin from serum samples.
- Hormone analysis: Introduction; Classification and general characteristics of hormones; Determination of cortisol from blood and urine samples; determination of oestrogens from urine samples

Food Product Analysis

- Moisture content, ash, fibre, nutrients, antinutrients, toxicants, microorganism-spoilage (rancid taste), colour, preservatives
- Analysis of amino acids, proteins, carbohydrates, lipids and fats
- Analysis of edible oils, dairy products, pickles etc., fruit and vegetable products
- Food additives and Food colours
- Food adulteration
- Sensory / organoleptic evaluation of food
- ISO 9000 and Food industry

Consumer Product Analysis

- Consumer products and their chemical speciation (as well as qualitative and quantitative analysis)
- Cosmetics – Face powders, hair preparations, Antiperspirants and deodorants, Perfumes, Toothpastes
- Food pigments

References:

1. B. M. Mittal and R. N. Saha, Handbook of Cosmetics, Vallabh Prakashan, New Delhi, 1st edn., 2000.
2. S. Nanda and R. K. Khar, Cosmetic Technology, Birla Publication Pvt. Ltd., 1st edn., 2006.

SEMESTER 4

DC-450: Industrial Products and Forensic Analysis (6 Credits) (72 Lectures)

Section I: (36 Lectures)

Industrial Products

- a. Steel and Ferrous Materials
- b. Cement and Building Materials
- c. Ceramic Materials
- d. Surfactants and Detergents
- e. Medicinal and Pharmaceutical Products
- f. Fertilizer Analysis

Section I: (36 Lectures)

- a. Analysis of Steel and ferrous materials:
Sampling, Analysis of steel and ferrous alloy: Carbon, silicon, manganese, phosphorous, sulphur, selenium, copper, nickel, chromium, vanadium, tungsten, molybdenum, cobalt, aluminium, titanium, nitrogen, lead, niobium, iron.
- b. Analysis of Cement and building materials:
Types of cement, sampling, Analysis of cement and building materials: Silicon dioxide, aluminium oxide, ferric oxide, calcium oxide, magnesium oxide, sulphur-trioxide, sulphide- sulphur, loss on ignition, insoluble residue, sodium and potassium oxide.
- c. Analysis of Ceramic materials:
Analysis of Quartz: Volatile residue, zirconium dioxide, aluminium oxide, calcium and magnesium oxides, sodium and potassium oxide.
Analysis of clays and feldspars: Determination of moisture, silicon dioxide, total oxides, ferric oxide, titanium dioxide, aluminium oxide, calcium oxide, magnesium oxide.
Analysis of glasses: Types of glasses, determination of lead and lead glass.

Analysis of ceramics: Determination of titanium dioxides and aluminium oxide from oxide ceramics.

Analysis of ferrous slags: Determination of iron, calcium and magnesium, total oxides.

d. Surfactants and Detergents:

Introduction to different terms, Classification, Representative methods of Analysis.

e. Water and effluent analysis:

Introduction to different terms, Classification, Representative methods of Analysis.

f. Soil and fertilizer analysis:

Introduction to different terms, Classification, Representative methods of Analysis.

Books:

1. "Standard methods of Chemical Analysis", Vol. 2, (Part A & B), F. J. Welcher, 5th edn., Von Nostrand & Robert E. Krieger Publishing Co. New York, (1975 and 2000).
2. "Quantitative Inorganic Analysis" A. I. Vogel, English Language Book Society, London, (1975).

Reference Book:

1. "Materials Science & Engineering, William D. Callister Jr., John Wiley and Sons, Inc. New York.,(1991).
2. "Encyclopaedia of Analytical Science", A. Townshend (Ed.), Academic Press (1995).
2. "Practical Pharmaceutical Chemistry, A. H. Beckett and J. B. Stenlake, CBS Publishers, New Delhi, 1st Indian edn., pp 16-76 and 309-348, (1986).

Section II: (36 Lectures)

Forensic Science

- a. **Forensic Analysis:** Overview, Destructive and Nondestructive techniques, Data interpretation.
- b. **Blood Analysis:** Blood preservation and ageing effects, Analysis of blood components and exogenic substances, blood stain analysis.
- c. **DNA Profiling :** DNA and its polymorphism, DNA typing procedures-RFLP, PCR, MVR-PCR, Dot-blot, AMP-FLP, STR, other methods, paternity testing, applications, interpretation and practical use.
- d. **Determination of alcohol in body fluids:** Legal background, Sampling and sample preservation, analysis-GC, IR, enzymatic and other methods.
- e. **Fingerprint analysis:** Latent fingerprints; optical, physical, physico-chemical & chemical detection methods; fingerprints in blood, fingerprint detection sequences.
- f. **Hair analysis:** Structure and composition of hair, morphological examination, Chemical analysis of hair components and components remaining on or in hair.
- g. **Systematic Drug Identification:** Classification and categories of compounds involved, analytical strategy-EMIT, FPIA, TLC, LC, GC-MS, etc., requirements for identification, possibilities & limitations of selected techniques, isotope detection method with numericals, new drug groups.
- h. **Materials of interest for Forensic studies: Explosives:** Types, analytical methods for identification of low and high explosives in post-blast debris. **Fibres:** Fibres encountered at crime scene, identification of types, dye extraction and analysis, colour matching, analysis for metals, additives and contaminants-SEM-EDX, XRD,XRF. **Paints, Varnishes and Lacquers :** Formulation of paints, types of sample, Sample pre-treatment prior to analysis, colour measurements, Analysis by SEM, SEM-SPMA, TEM, TLC/HPTLC, PyrGC, IR, Raman, UV-Vis-Flu, XRF, AES, TG-DTA. **Glass :** As forensic evidence, measurement of physical properties, elemental analysis-XRD, NAA, etc., interpretation of results, casework examples. **Arson Residues :** nature of arson evidence, chemical evidence, properties of liquid accelerants, sampling and

sample pre-treatment, laboratory examination of suspect arson evidence, evidential value. **Gunshot Residues** : Composition of sources, detection on hands & its limitations, determination of muzzle-to-target distance, elemental & inorganic analysis, numericals on estimation of energy released by combustion reactions, etc.

References :

1. 'Forensic Chemistry' by Suzanne Bell, Pearson Prentice Hall Publishers, 2006
2. Encyclopaedia of Analytical Chemistry, Volume 3, Academic Press, 1995

DC-451: Environmental Chemistry (6 Credits) (72 Lectures)

Water : Sources of water, human use, type and sources of impurities, water quality parameters and standards, sampling, preservation and chemical speciation, physical analysis of water: color, pH, temperature, specific conductance, odour and taste, transparency and turbidity detection, Chemical Analysis of water : Total dissolved solids, Dissolved oxygen, total hardness, total alkalinity, chloride, fluoride, sulphate, sulphide, phosphate, boron, nitrogen, COD, BOD, total organic carbon, phenol, pesticides, tannin and lignin, E. coli and total bacteria, rain water harvesting.

Air : Natural and anthropogenic sources of pollution, primary and secondary pollutants, transport and diffusion of pollutants, gas laws governing the behaviour of pollutants in the atmosphere. Methods of monitoring and control of air pollution SO₂, NO_x, CO, H₂S, SPM. Effects of pollutants on human beings, plants, animals, materials and on climate, Auto exhaust emission-characterization and analysis, analysis of particulate matter, Instrumental techniques for air pollutants, spectrophotometric analysis of gaseous air pollutants, thermochemical and photochemical reactions in the atmosphere, oxygen and ozone chemistry, chemistry of air pollutants, photochemical smog, Acid rain, air quality standards.

Soil : Composition, water, air, inorganic and organic components, micro and macro nutrients pollutants in soil, acid base and ion exchange reactions in soil, collection and preparation of soil samples for analysis, solid texture estimation, determination of rheological properties and electrical conductivity of soil, soil pollution control, industrial waste effluents and heavy metals, their interaction with soil components, soil micro-organisms and their functions, degradation of different insecticides, fungicides and weedicides in soil, different types of synthetic fertilizers and their interaction with different components of soil, determination of CO₃²⁻, HCO₃⁻, Cl⁻, SO₄²⁻, Ca²⁺, Mg²⁺, Na⁺, K⁺.

Noise : Sources of noise pollution, measurement of noise and indices, effect of meteorological parameters on noise propagation, noise exposure levels and standards, noise control and abatement measures, impact of noise on human health.

Sources of Energy : Sun as source of energy, solar radiation and its special characteristics, fossil fuels-classification, composition, physico-chemical characteristics and energy content of coal, petroleum and natural gas, principles of generation of hydroelectric power, tidal. Ocean thermal ocean conversion, wind, geothermal energy, solar collectors, photovoltaics, solar ponds, nuclear energy-fission and fusion, magneto hydrodynamic power, bio energy-energy from biomass and biogas, anaerobic digestion, energy use pattern in different parts of the world.

Environmental implication of energy use, CO₂ emissions, global warming, air and thermal pollution, radioactive waste and radioactivity from nuclear reactors, impacts of large-scale exploitation of solar, wind, hydro and ocean energy.

Chemical toxicology and metal toxicology : highly toxic solids, liquids and gases, biochemical effects of toxic metals on man, mercury, lead, cadmium, arsenic, vanadium, chromium, cobalt, asbestos, carcinogenic compounds poisoning, diagnosis, effects and treatment.

Effluent Analysis : Effluent treatment and legislation, characterization of waste water, classification of effluents, waste water treatment processes and recycling, analysis of waste water, physical methods of characterization, analysis of organic and inorganic pollutants, automation in effluents analysis.

References

- 1) Environmental Chemistry: M.Satake, Y.Mido, Editors: S.A.Iqbal, M.S. Setthi, Discovery publishing house (1994).
- 2) Environmental Chemistry: A.K.De, Wley Interscience (1993)
- 3) Environmental Chemistry: B.K. Sharma and H. Kaur, Goel Publishing house (1997)
- 4) Ecology, Chemistry and Management of Environmental Pollution: M.C. Dash, published by Macmillian India Ltd., (2004)
- 5) Water and Wastewater Technology: Mark J. Hammer, Mark J. Hammer, Jr. (2001)

DC-454: Biosensors and Agrochemicals (4 Credits) (48 Lectures)

Section I: Biosensors (2 Credits)

Biosensors

- Definition, components and types of Biosensors
- Enzyme-based Biosensors
- Immobilization of enzymes
- Types of transducers, fabrication of probes for sensors and evaluation of sensor performance
- Applications of Biosensors

References:

1. A. Townshend, Ed., Encyclopedia in Analytical Science, Academic Press (1995)
2. R. L. Na Academic Press, Calcutta .

Section II: Agrochemicals / Organic Polymers and Agrochemicals (2 credits)

Organic Polymers

Basic concepts:

Polymers, monomers, Molecular weight and molar mass, End groups, Degree of polymerization, Nomenclature Classification of polymer-thermoplastic, thermosetting Copolymers- random, alternate, block and graft copolymers

Molecular architecture

Polymerization and functionality

Polymerization processes- Addition and step polymerization

Mechanism of polymerization – free radical and ionic. Heterogeneous polymerization – Zeigler-Natta catalysis.

Optically Activity in Polymers, Stereo isomers – isotactic, atactic and syndiotactic polymers

Analysis of Polymers

Molecular Weight of polymers – Arithmetic, weight average and number average molecular weights of polymers

Determination of molecular weight of polymers

End-Group Analysis

Cryoscopy, Light scattering, Viscosity, and gel permeation chromatographic methods.

Thermal Transition in Polymers

T_g and T_m and their relation, DSC, TGA

Spectral methods of Analysis

Analysis of Agrochemicals:

Introduction, Classification, mechanism of action and synthesis.

Insecticides : DDT, BHC, Aldrin, Endosulfon, Malathion, Parathion.

Herbicides : 2,4-dichloro phenoxy acetic acid, dalapon, paraquat, Banalin, Butacarb .

Fungicides : Boardeaux mixture, Copper oxychloride, Zineb,, Benomyl(Benlte)

Analysis of pesticide residue and toxicological effects.

Books:

1. Text Book of Polymer Science by F. W. Bilmayer;
2. Polymer Science by Gowarikar
3. Introduction to polymer science and chemistry by Manas Chanda, Taylor and Francis Pub.
4. Chemistry of pesticides, N.M. Melnikov, Residue Reviews, Vol.36, Springer Verlag, New York , 1971.
5. Future for insecticides , R.C. Netealr, J.J.Mckalvery, Jr. John Wiley & Sons, New York, 1976.
6. Pesticide processes Encyclopedia, Marshal Sitting Hoyes Data Corporation, U.S.A., 1977.

OR

Surfactant, Elemental Analysis.

Dye and pigments

Dyes and Pigments:

- (a) Introduction to different terms, Classification, Representative methods of Analysis.
- (b) Surfactants and Detergents: Introduction to different terms, Classification, Representative methods of Analysis.

(c) Medicinal and Pharmaceutical Products: Introduction to different terms, Classification, Representative methods of Analysis.

Text Books:

1. "Standard Methods of Chemical Analysis", F. J. Welcher, 5th edn., Von Nostrand (2000).

References:

1. "Encyclopaedia of Analytical Science", A. Townshend (Ed.), Academic Press (1995).
2. "Practical Pharmaceutical Chemistry", A. H. Beckett and J. B. Stenlake, CBS Publishers, New Delhi, 1st Indian edn., pp 16-76 and 309-348, (1986).

OR

Pharmaceuticals and Petrochemicals .

M. Sc. Semester III (Analytical Chemistry) Practical Courses

Course DC-358: Analytical Chemistry Practicals I (4 credits, ~ 7.5 weeks)

A. Practicals to be conducted by Inorganic Chemistry Section: (Any six experiments)

(3 weeks) = (12 days)

1. Alloy [e.g. iron, chromium and nickel from Stainless steel]
2. Ore [e.g. acid-insoluble matter (combined oxides), iron and titanium from Ilmenite]
3. Cement [e.g. silicon, aluminium, iron from Portland cement]
4. Consumer products (e.g. Inorganic Pigment [e.g. chromium from Zinc chrome]; Pharmaceutical product [magnesium from tablet of “Milk of magnesia” / calcium from calcium-supplementary tablet / aluminium from alum]; Fertilizer [NPK Fertilizer for phosphorus]
5. Ion exchange chromatography [separation and estimation of mixture of zinc (II) and magnesium (II)]
6. Thermogravimetry [Determination of percentage of $MgCO_3$ in Dolomite]
7. Flame Photometry [Determination of the percentage of sodium in the sample of dairy whitener]
8. Cyclic voltametry [Study of cyclic voltammogram of $K_3[Fe(CN)_6]$]
9. Determination of moisture content in food sample using Karl-Fischer Titrator
10. Determination of Phosphate in Detergents by Spectrophotometry
11. Determination of phosphoric acid in cola beverages by pH titration.
12. Photometric Titrations: (a) Cu Vs EDTA (b) Fe Vs EDTA using salicylic acid
13. Potentiometric Titrations: (a) FAS Vs $K_2Cr_2O_7$ (b) FAS Vs. $KMnO_4$
14. Conductometric Titrations: (a) NaOH Vs. HCl (b) NaOH Vs. Boric acid
15. Synthesis of semiconducting nano oxides such as NiO, ZnO
16. Table work for IR-spectra, NMR, UV-Visible spectra

References

1. A. I. Vogel, A textbook of Quantitative Inorganic analysis, 2nd edn., ELBS edn.

2. Pharmacopoeia of India.

**B. Practicals to be conducted by Physical Chemistry Section: (Any six experiments)
(3 weeks) = (12 days)**

1. Fluorometric determination of Riboflavin (Vitamin B2)
2. Determination of quinine in commercial soft drink by molecular fluorescence spectroscopy
(Analytical Chemistry-6th Ed. G. D. Christian page no. 775)
3. Molecular weight of polymer from Viscosity measurements
(Experiments in physical chemistry- J. M. Wilson and others page no. 202)
4. Determination of activity coefficient of an electrolyte / non-electrolyte by cryoscopy
(Experiments in physical chemistry- J. M. Wilson and others page no. 150 & 153)
5. Differential potentiometric titration
(Experiments in physical chemistry- J. M. Wilson and others page no. 272)
6. Kinetic Methods of Analysis: Enzymatic Determination of Glucose
D. A. Skoog, D. M. West, F. J. Holler, and S. R. Crouch, *Analytical Chemistry: An Introduction*, 7th ed., Chapters 21 and 22, pp. 547-592
7. TGA for a mixture of CuSO₄ and NaCl, find out the percentage of each constituent in the mixture.
8. Estimation of Zn and Cd from their mixture by polarographic technique

Each experiment includes standardization of the reagents, calibration of the instrument with known reagents and analysis of an unknown.

References

- a. A. I. Vogel, A textbook of Quantitative Inorganic analysis, 2nd edn., ELBS edn.
- b. A. I. Vogel, A textbook of Practical Organic Chemistry, 4th edn., ELBS edn.
- c. Pharmacopoeia of India.

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Course DC-359: Analytical Chemistry Practicals II (4 credits, ~ 7.5 weeks)

A. Practicals to be conducted by Organic Chemistry Section: (Any six experiments)

(3 weeks) = (12 days)

1. Estimation of Tannin from tea
2. Isolation of caffeine from tea
3. Quantitative analysis of mixture by gas Chromatography [e. g. Chloroform and carbon tetrachloride / methanol and ethanol]
4. Preparation of sulphanilamide from acetanilide and assay its purity
5. Preparation of methyl salicylate and assay its purity
6. Isolation of Lycopene from tomato / β -Carotene from carrots and assay its purity
7. Preparation, purification and assay of aspirin.

Note: All organic compounds used as drugs prepared here will be purified and assayed for purity by standard IP / BP / VSP methods.

References

1. A. I. Vogel, A textbook of Practical Organic Chemistry, 4th edn., ELBS edn.
2. R. Ikan, Natural Products.

B. Practicals to be conducted by Biochemistry Section: (Any six experiments)

(3 weeks) = (12 days)

1. Determination of glucose from blood serum (Enzyme method)
2. Determination of cholesterol & HDL from blood serum by kit method / colorimetry
3. Estimation of urea from blood sample (kit method)
4. Determination of glucose from blood serum by Folin –Wu – method
5. Assay of Thiamine
6. Assay of polymers and plastics
7. Estimation of Ketone bodies
8. Estimation of Creatine / Creatinine in urine

9. Estimation of total carbohydrates by Anthrone method.

References

1. A. I. Vogel, A textbook of Practical Organic Chemistry, 4th edn., ELBS edn., ().
2. H. Varley, Practical Clinical Biochemistry, 4th edn., CBS Publishers and Distributors, New Delhi ().

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Course DC 458 : Project Work 7 credits