M Sc-II Inorganic chemistry
Semester III and IV Courses

Compulsory courses			**Optional courses**		
Code	**Title**	**Credits**	**Code**	**Title**	Credits
CHIC 501	Coordination and organo-metallic chemistry	**4**	**CHIO 501**	Bioinorganic Chemistry	**4**
CHIC 502	Solid State Chemistry	**4**	**CHIO 502**	Catalysis: Fundamentals and Chemical concepts	**4**
CHIC 503	Group Theory and Spectroscopy	**4**	**CHIO 503**	Chemistry of Main Group Elements	**4**
CHIC 504	Experiments in Inorganic Chemistry	**4**	**CHIO 504**	Topics in Inorganic Chemistry	**4**
			CHIO 505	Laboratory Course in Inorganic chemistry –I	**4**
			CHIO 506	Laboratory Course in Inorganic chemistry –II	**4**
			CHIO 507	Dissertation	**8**

CHIC – 501 COORDINATION AND ORGANOMETALLIC CHEMISTRY

(4 Credits)

1. Coordination Chemistry: 1.1 Bonding in coordination compounds; i) valence bond theory, VBT; ii) Crystal field theory and iii) Molecular orbital theory. (20)
1.2 Spectra: i) Electronic spectra of coordination compounds; ii) Use of IR spectroscopy in coordination compounds. (15) 1.3 Magnetism: Magnetic Properties of metal complexes; paramagnetism, diamagnetism, ferromagnetism, antiferromagnetism, spin cross over phenomenon, temperature independent paramagnetism; Curie law, Curie-Weiss Law. (10) 1.4 Structure: Structure of coordination compounds with coordination number 1 to 8; examples of higher coordination numbers; isomerism in coordination compounds- linkage isomerism, chelate effect (10)
1.5 Reaction Mechanism: Reaction mechanism in coordination compounds; thermodynamic and kinetic stability, equilibrium constants, formation constants, lability, inert complexes, kinetics of substitution reactions in octahedral and square planar complexes, trans effect – theories of trans effect, atom transfer reactions; electron transfer reactions- inner sphere mechanism, outer sphere mechanism, Frank Condon principle, Marcus equation (20)
2. Organometallic chemistry: 18- electron rule, effective atomic number, metal carbonyls, metal nitrosyl compolexes, dinitrogen complexes, types of M-C bonds, reactions of organometallic complexes, homogenous catalysis by organometallic compounds, stereochemically rigid molecules (25)

Note: Numbers in bracket indicate percent weightage

Reference books:

1. J. E. Huheey, E.A. Keiter and R. L. Keiter, "Inorganic Chemistry: Principles of structure and reactivity", 4th Edition, Addison Wesley Publ. Co. 1993 (Chapter 11, 12, 13 and 15)
2. F. A. Cotton, G. Wilkinson and P.L. Gaus, "Basic Inorganic Chemistry", 3rd Ed., John Wiley 1995.
3. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry" 3rd Ed. Wiley Eastern, New Delhi 1984 (4th and 5th eds. preferred)
4. D. F. Shriver and P.W. Atkins "Inorganic Chemistry" 3rd Ed., Oxford University Press, 1999
5. D. Banerjea, "Coordination Chemistry" Tata McGraw – Hill, New Delhi 1994
6. N. N. Greenwood and A. Earnshaw, "Chemistry of the Elements" Pergamon Press, Exeter, Great Britain 1984.
7. J. D. Lee, "Concise Inorganic Chemistry", 5th ed. Chapman and Hall, 1996.
8. G. Rodgers, "Introduction to coordination, solid state and descriptive Inorganic chemistry" McGraw – Hill 1994

CHIC-502 Solid State Chemistry (4 Credit)

1. Structure and bonding (12)

Crystal lattice; Unit Cell; Miller indices and planes; X-ray diffraction method; Molecular solids; Hydrogen bonding, metallic, covalent and ionic solids; structural classification of bianary and tertiary compounds, Determination simple structure; spinel and perosvskite structures.

2. Non Stoichiomestry in solids: (6)

Oxygen deficient Oxide, Metal deficient Oxides, and classification of non-Stoichiometry.

3. Crystal defects: (8)

Point defects; Schottky and Frenkel defects; Dislocations, plane defects and line defects;

4. Preparation Techniques (20)

Ceramic and different wet Chemical methods; single crystal: i) growth from melt, ii) From solution, flux method, iii) Epitaxial growth of single crystal thin films, iv) Chemical vapour transport, v) Hydrothermal and dry high pressure methods; arc technique; Thin films: physical and chemical method; Amorphous materials; Nanoparticle solids : Different methods of preparation, properties and applications.

5. Reactions of Solids: (8)

Tarnish reactions, decomposition reaction, Solid-Solid reactions, addition reactions, double decompositions reaction, electron transfer reaction, Solid-gas reactions, Sintering, factors influencing reactiviy of Solids.

6. Phase Transformations in Solid: (10)

Thermodynamic consideration, Burgers classifications, structural change in phase transformation, Mantensite transformation, Temperature and pressure induced transformations, Order- disorder transitions, Electronic transition, Transformation with a change in composition, Enantiotropy and monotropy, Ehrenfest's classification.

7. Electrical Properties (12)

Electrical conductiviy, Free Election Theory, Fermi energy, Insulators, Semiconductor and conductors, Band theory of semiconductor, Brilliouin zones, Hall effect, the Seebeck effect, Photo conductivity, Ionic conductivity, superconductivity, BCS theory, Meissner effect, high temperature superconductor.

8. Semiconductor Devices: (8)

Diodes and transistors, Junction field effect transistor and metal Oxide semiconductor field effect transistor, Photo sensitive devices, light meter, Photodiode, Phototransistor, Solar cells, light emitting diodes, laser materials.

9. Optical, dielectric and thermal properties: (8)

Luminescence and phosphorescence, piezoelectronic, feroelectronic materials and applications, Thermal conductivity, phonon interaction, thermal expansion coefficient.

10. Magnetic properties: (8)

Introduction to magnetism, behavior of substance in a magnetic field, magnetic moments, Diamagnetism, Paramagnetism, Experimental determinations of susceptibility, Ferromagnetism, Antiferromagnetism, Ferrimagnetions, Magnetizations of a ferromagnetic substance.

Note: Numbers shown in bracket is the percentage weightage.

REFERENCE BOOKS:

1. L. V. Azaroff, “Introduction to solids” (Tata McGraw Hill)
2. N. B. Hannay, “Solid State Chemistry” (Prentice Hall)
3. H. V. Keer, “Principles of the Solid State” (Wiley Eastern Ltd, New-Delhi)
4. C. N. R. Rao, “Solid State Chemistry” (Dekker New Yark)
5. C. N. R. Rao and K. J. Rao, “Phase Transitions in Solid” (McGraw Hill)
6. A. R. West, “Solid State Chemistry” (John Wiley and Sons) 2005.
7. W. D. Callister, “Material Science and Engineering: An Introduction” John Wiley, New York (1985)
8. D. K. Chakraborty, “Solid State Chemistry” (New Age International Publishes, 2010).

CHIC – 503 GROUP THEORY AND SPECTROSCOPY (4 Credits)

1. Group Theory: Basic definations and theorems of group theory, Molecular symmetry and the symmetry groups, symmetry elements and operations, symmetry planes and reflections, inversion center, proper axes and proper rotations, imporoper axis and improper rotations. Products of symmetry operations, equivalent symmetry elements and equivalent atoms, symmetry point groups, systematic symmetry classification of molecules, classes of symmetry operantions, representations of groups, some properties of matrices and vectors, reducible and irreducible representations, properties of the characters of representations, character tables, group theory and quantum mechanics, wave functions as basis for irreducible representations, direct product, space groups, translational symmetry. (40)

1.1Symmetry aspects of molecular orbital theory, general principles, the secular equation, the Huckel approximation, simple LCAO-MO theory of homocyclic π systems. More general cases of LCAO-MO pi-bonding, Molecular orbitals for the metal sandwich compounds. (10)

2. Spectroscopic Methods: Magnetic Resonance Spectroscopy, interaction between electron / nuclear spin and magnetic field, presentation of ESR spectrum, hyperfine splitting, (e.g. H atom, methyl radical etc.), number of expected ESR signals for 1 electron paramagnetic species, zero field splitting and kramer's degeneracy, Spin energy levels of octahedral Mn(II) complexes, nuclear quadrupole interaction, spin Hamiltonian, ESR line widths, Electron delocalization, ESR instrumentation, NMR spectral discussion of a few nuclei like 19F and 31P, Mossbauer spectroscopy; Mossbauer effect, principles of Mossbauer spectroscopy, Mossbauer line widths, Doppler shift, experimental arrangement of Mossbauer spectroscopy, chemical shift (isomer shift), quadrupole splitting, Magnetic heperfine interaction; use of IR as tool in the structure determination of coordination complexes. (40)

3. Solid State and surface Spectroscopy: Electronic spectroscopies of surfaces: XPS and AES (10)

Note: Numbers in bracket indicate percent weightage.

Reference Books:

1. F. A. Cotton, Chemical Applications of Group theory" Wiley Eastern, New Delhi, 1976.
2. P.W. Atkins, "Physical Chemistry", 5th Ed., W. H. Freeman and co., New York 1994 (chapters 15, 17, 18)
3. R. L.Dutta and A. Syamal, "Elements of Magnetochemistry", 2nd Ed. Affiliated East-West Press, New Delhi (1993)
4. C. N. Banwell and E. M. McCash, "Fundamentals of Molecular Spectroscopy", 4th Ed., Tata McGraw Hill, New Delhi 1994
5. R. S. Drago, "Physical Methods in Inorganic Chemistry" Affiliated East – West Press 1978
6. E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, "Structural Methods in Inorganic Chemistry" ELBS 1988

CHIC – 504 EXPERIMENTS IN INORGANIC CHEMISTRY (4 credit)

Group – 1: Experiments in coordination chemistry: Ligand and complex synthesis, metal analysis (35)

1) Purification (distllation/rycrystallisation) of ligands like acacH, en, carboxylic acids etc,
2) Preparation of manganic tris(acetylacetonate) and estimation of Mn
3) Preparation of tris(thiourea)copper(I)sulfate and estamation of Cu
4) Preparation of isomers; cis and trans-dichloro(ethylenediamine)cobalt(III)chloride and estimation of cobalt
5) Preparation and resolution of tris(ethylenediamine)Cobalt(III) ion and estimation of chloride
6) Preparation of cis and trans-potassium dioxalatodiaquochromate(III) and estimation of chromium
7) Preparation of nitro and nitrito-penta aminecobalt(III)chlorides and estimation of cobalt
8) IR spectral characterization of free ligands and coordinated ligands

NOTE: In complex synthesis, the student is expected to recrystallise the product, record IR spectra and carry out metal analysis. Spectral analysis can be carried over.

Group –2 Experiments in Solid state chemistry (35)

1) Preparation of spinel oxides by precursor method 2) Estimation of metals in precursors and oxides, 3) Characterization of precursors by thermal analysis 4) Characterization of precursors and oxides by infrared analysis 5) Characterization of precursors and oxides by chemical analysis 6) X-ray diffraction studies of oxides

Electrical characterization: 7) direct current electrical resistivity of semiconductor (Ge/Si) by Four Probe 8) Curie temperature determination of dielectric material (PZT) by measurement of dielectric constant v/s temperature, 9) Measurement of saturation magnetization, Ms, Mr and Hc, 10) Determination of curie temperature of magnetic oxides by a.c. susceptibility studies.

Group – 3: Instrumental methods / spectral analysis /ion exchange (15)

Determination of stability constant of complex ions in solution

1) Fe(III) – salicylic acid complex (Job's Method)
2) Fe(III) – thiocyanate complex 3) Fe(II) – 1,10-phenanthroline
4) Determination of instability constant for the reaction between Ag^+ and NH_3
5) Determination of instability constant for the reaction between Ag^+ and en
6) Determination of instability constant for the reaction between Cu^{2+} and NH_3
7) Determination of instability constant for the reaction between Cu^{2+} and en

Ion exchange chromatography:

8) Separation of Mg^{2+} and Co^{2+} by anion exchange column
9) Separation of transition metal cations by anion exchange column

Group – 4: Ore / Alloy/ commercial sample analysis (15)

1) Analysis of Goan Iron ore: Hematite / magnetite

2) Analysis of Devardas alloy
3) Analysis of solder (Pb and Sn)
4) Analysis of calcite

Reference Books:

1. G. Brauer "Handbook of Preparative Inorganic chemistry" 2nd ed., Vol. 1 and 2, Academic Press New York 1967.
2. J. Bassett, R.C. Denny, G. H. Jeffery and J. Mandham, "Vogel's Text Book of Quantitative Inorganic Analysis" 4th ed. ELBS 1985.
3. G. Marr and B. W. Rockett, "Practical Inorganic Chemistry", Van Nostrnad Reinhold London 1972.
4. G. Pass and H. Sutcliffe, "Practical Inorganic Chemistry" 2nd Ed. Chapman and Hall 1985.
5. J. D. Woolins, "Inorganic Experiments" Wiley – VCH Verlag GmbH and Co, 2003

CHIO – 501 BIOINORGANIC CHEMISTRY (4 credits)

1. Essential elements in biology, distribution of elements in biosphere, bio-availability, bio-stability, building blocks of the biosphere; namely sugars (carbohydrates), fatty acids (lipids), nucleotides (nucleic acids) and amino acids (proteins), Biological importance of water, and brief review of the chemistry of biopolymers. Metallobiomolecules: classification of metallobiomolecules, metalloprotiens (enzymes), metal activated proteins (enzymes), role of metal in metal protein systems, Principles of coordination chemistry related to bioiorganic research, physical methods in bioinorganic chemistry (30)
2. Alkali metal and alkaline earth metal cations in biology, introduction, biological importance of the alkali and the alkaline earth cations, Cation transport through membranes (ion pumps). Photosynthesis, Hill reaction, Chlorin macrocycle and chlorophyll, Absorption of light by chlorophyll, role of metals in photosynthesis, in vitro photosynthesis. (15)
3. Non redox metalloenzymes, zinc metalloenzymes like carboxypeptidase, carbonic anhydrase and alcohol dehydrogenase, Bio-functions of zinc enzymes, active site structure and model complexes. Oxygen carriers and oxygen transport proteins, iron porphyrins (Haemoglobin and myoglobin). Haemocyanins and Haemerythrins, Synthetic models for oxygen binding haemprotiens. (20)
4. Biological redox reactions, haemprotiens cytochrome 'c', catalase peroxidase, and superoxide dismutase, blue copper proteins, vitamin B_{12} conezymes, nitrogen fixation and iron-sulfur proteins, biological nitrogen fixation, nitogenase and dinitrogen complexes, iron-sulfur proteins, synthetic analogues for Fe-S proteins, core extrusion reactions. (20)
5. Metal transport and storage: A brief review of iron transport and storage, transferring, ferritin and siderphores. Therapeutic uses of coordination compounds (10)
6. Synthesis of a few ligands for modeling the metalloactive sites of metallobiomolecules (this will involve both collection of synthetic procedures from library, term paper presentation/discussion (5)

Note: Numbers in bracket indicate percent weightage.

Reference books:

1. R. W. Hay, "Bioinorganic chemistry", Ellis Horwood Chichester, 1984
2. M.N. Hughes, "The Inorganic Chemistry of Biological process" 2nd Ed., Wiley (Intersciences) New York, 1984
3. S. J. Lipard and J. M. Berg, Principles of Bioinorganic chemistry, panima Publishing Corporation
4. E. E. Conn, P.K.Stumpf, G. Bruening and R. H. Doi, "Outlines of Bioinorganic chemistry", 5th Ed Wiley Eastern, New Delhi, 1983
5. B. I. Britini, H. B. Gray, S. J. Lippard and J. S. Valentine, "Bioiorganic chemistry", University Science books, Mill Valey, CA, 1994.
6. D. E. Fenton, "Biocoordination Chemistry", Oxford Chemistry Printers, 25 Oxford University Press 1995

CHIO-502 CATALYSIS: FUNDAMENTALS AND CHEMICAL CONCEPTS

(4 credit)

1. **Origin and development of catalysis**: (6)

Differences between heterogeneous, homogeneous, auto and bio-catalysts; Importance of heterogeneous and homogeneous catalysis in chemical reactions and in industries.

2. Heterogeneous Catalysis **(**44)

(i) Adsorptions: Physical and chemical adsorption, chemisorptions of gases on solid surfaces, nature of adsorbed layer, dissociative adsorptions, models is chemisorptions , scattering, trapping and sticking, simple adsorptions isotherm, Langmuir adsorption, the BET adsorption isotherm.

(ii) Types of Catalysis: Preparations and separations of the Catalysts, Meso and micro porous materials, nano material catalysts and significance zeolites and related molecular sieves, supported and bifunctional catalysts. Activity and life of the catalysts, active centers, promoters and poisons, catalyst deactivations.

(iii) Characterization of Solid Catalysts: Surface area, , stucture and surface morphology, porosity, pore volume and diameter, particle size, X-ray diffraction , SEM, TEM, x-ray absorption spectroscopy, XPS and Anger Spectroscopy to surface studies, TPD, TPR for acidity and basicity of the catalysts.

(iv) Heterogeneous reactions: Thermodynamic consideration in surface reactions, ammonia synthesis, oxidation reduction reactions (selected examples), synthesis of methonal, fisher trophs catalysis, selective catalytic reduction, mechanism of catalytic reactions, method of finding rate of the reactions and the rate determining steps.

(v) Theories of Catalysis : Boundary layer theory, Catalysis by semiconductors, Wolkenstein theory, Balanding's approach, electronic factors is catalysis by metals, molecular orbital approach.

3. **Homogeneous Catalysis** **(**14)

Inter mediate stages in homogenous Catalysis, energy profile diagram, general scheme for calculating kinetics of reactions, decomposition of hydrogen peroxide, acid-base catalysis, hydrogenation, hydroformulation, isomenization and wacker reaction, C-C bond forming reactions and asymmetric oxidations.

4. **Bio-catalysis** (6)

Enzyme catalysis reactions (selected few examples), Immobilized enzymes and cells, catalytic antibodies.

5. **Catalytic polymerizations** (6)

Homogeneous and heterogeneous catalysis is polymerizations reactions (few examples), Ziegler – Natta catalyst in is polymerizations reactions.

6. **Photocatalysis** (6)

Porphyrins, phthalocyanes and semiconductor as photo catalysts in photolysis reactions

Generation of hydrogen by photo catalysts, photocatalytic break down of water and harnessing solar energy.

7. **Phase transfer catalysis**- (6)

Basics and types of phase transfer catalysis, selected examples.

8. **Practical demonstrations, practical exercise and term paper presentations** (12)

REFERENCE BOOKS:

1. P. H. Emmett, “Catalysis” (Vol I) (Reinhold, New York)
2. D. K. Chakraborty, “Adsorption and catalysis” (Wiley Eastern Ltd)
3. J. M. Thomas and W.J. Thomas “heterogeneous catalysis” (VCH publication 1997).
4. A. Clark, “The Theory of adsorption and catalysis” (Academic press)
5. E. R. Rideal, “Concept in Catalysis” (Academic press)
6. G. M. Panchenov and V. P. Lebedev, “Chemical kinetics and catalysis” (Mir publication).
7. Baker, “Novel material in heterogeneous catalysis”
8. S. J. Thomson and G. Webb, “Heterogeneous Catalysis” (Oliver and Boyd Publications)
9. R. A. Van Santen and J. W. Niemantsvedict, “Chemical Kinetics and Catalysis (Plenum Press).

CHIO-503 CHEMISTRY OF MAIN GROUP ELEMENTS (4 credits,)

1. Hydrogen and the hydrides (5)

1.1 Hydrogen: Electronic structure, position in periodic table, abundance, preparation, properties, isotopes, ortho and para hydrogen, coordination chemistry of hydrogen.

1.2 Hydrides: Classification, preparation, properties; Hydrogen ion, hydrogen bonding and its influence on properties.

2. General properties and its Trends in groups and periods and Group 1 Elements (10)

Group 1 Elements: Introduction, abundance, extraction, physical and chemical properties, solubility and hydration, solutions of metal in liquid ammonia, complexes, crowns and crypts, electrides, alkalides, biological importance of Na and K, difference between lithium and the other group 1 elements, diagonal relationship.

3. Group 2 Elements (10)

Introduction, abundance, extraction, physical and chemical properties, solutions of metal in liquid ammonia, complexes, anomalous behaviour of beryllium, difference between beryllium and the other group 2 elements, diagonal relationship, biological importance of Mg and Ca. Grignard reagent: Preparation and properties.

4. Group 13 Elements (16)

4.1 Introduction, abundance, extraction of B and Al, physical and chemical properties, uses, complexes, difference between boron and the other group 13 elements, diagonal relationship.

4.2 Preparation, bonding and structure: Higher boranes; borane anions, carboranes, metallocarboranes, borates, boron nitride.

5. Group 14 Elements (10)

5.1 Introduction, abundance, physical and chemical properties, uses.

5.2 Carbon dating, graphite, graphene, metallocarbohedrenes, freons, organosilicon compounds, cluster compounds of Ge, Sn and Pb.

6. Group 15 Elements (12)

6.1 Introduction, abundance, physical and chemical properties, uses.

6.2 Compounds of phosphorous: oxides, oxoacids, sulphides, oxosulphides, organo-phosphorous compounds.

7. Group 16 Elements (15)

7.1 Introduction, allotropes of S, Se, Te, physical and chemical properties, uses.

7.2 Preparation, properties and structure of compounds: oxides, oxoacids, oxohalides, halides, hydrides.

7.3 Polyatomic sulphur cations, anionic polysulphides, compounds with sulphur as ligand;

7.4 Sulphur-nitrogen and sulphur-nitrogen-oxygen compounds.

8. Group 17 Elements (14)

8.1 Introduction, physical and chemical properties and uses.

8.2 Preparation and structure of compounds: oxides, oxoacids, oxohalides, halides, halogenoxide fluorides and related compounds.

8.3 Preparation and structure of radicals: polyhalide anions, polyhalonium cations, halogen cations,

9. Group 18 Elements **(08)**

9.1 Introduction, physical properties, clathrates.

9.2 Preparation, properties and structure of xenon compounds, compounds of other noble gases.

Reference Books:-

1) N. N. Greenwood and A. Earnshaw, 'Chemistry of the elements', 2nd Edition, Butterworth-Heinemann, Oxford, 2005

2) J. D. Lee, 'Concise Inorganic Chemistry', 5th Edition, Wiley India (P) Ltd., New-Delhi, 2003

3) J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, 'Inorganic Chemistry: Principles of structure and reactivity', 4th Edition, Dorling Kindersley (India) Pvt. Ltd., Delhi, 2008

4) P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, 'Inorganic Chemistry', 4th Edition, Oxford University Press, New-Delhi, 2008

CHIO – 504 TOPICS IN INORGANIC CHEMISTRY (4 Credits)

1. **Chemistry of d and f-block elements**: Introduction to d-block elements, Periodic properties of 3d/4d/5d elements, frost diagram and variable oxidation states, structural trends down the groups, mononuclear oxo complexes of iron, ruthenium, chromium, etc., nitride and alkylidyne complexes, polyoxometallates, intermediate oxidation states, metal-metal bonded d-metal complexes, noble character, metal sulfides and sulfide complexes; Introduction to f-block elements- periodic properties of lanthanides and actinides, differences between the 4f and 5f orbitals, absorption spectra of lanthanides and actinides, lanthanide chelates, transactinide elements. (20)

2. **Compounds of Nitrogen and Oxygen**: Compounds of nitrogen, general remarks, nitrogen hydrides, ammonia, hydrazine, hydroxylamine, oxides of nitrogen, oxyacids and anions of nitrogen, dinitrogen and nitrogen compounds as ligands in coordination chemistry; Compounds of Oxygen; general remarks, stereochemistry of oxygen compounds, properties of dioxygen molecule, oxygen fluorides, hydrogen peroxide, peroxo compounds, superoxides, ozonides, oxygen compounds as ligands in coordination chemistry. (30)

3. **Fundamentals of Inorganic Electrochemistry and corrosion**: Basic aspects of electrochemistry, electron transfer reactions at electrode surface, potential and electrochemical cells, voltammetric techniques, linear voltammetry, cyclic voltammetry; reversible, irreversible and quasireversible processes; applications of cyclic voltammetry with reference to ferrocenes, transition metal complexes, Corrosion: Response of material to chemical environments, Galvanic corrosion and other forms of corrosion (25)

4. **Applications of Inorganic compounds**: Active complexes: Platinum Anticancer drugs contrast agents for X-ray and NMR imaging, ruthenium complexes, antiperspirants. Active elements: Lithium drugs, gold antiarthritic drugs, silver and mercury antimicrobial agents. Active ligands: Antihypertensive agents, nitric oxide as muscle relaxant, anticancer agents, antiviral agents, metal chelation by organic drugs, metalloenzyme inhibitors. (25)

Note: Numbers in bracket indicate weightage percent.

Reference Books:

1. D. F. Shriver and P.W. Atkins "Inorganic Chemistry" 3rd Ed., Oxford University Press, 1999

2. J. E. Huheey, E.A. Keiter and R. L. Keiter, "Inorganic Chemistry: Principles of structure and reactivity", 4th Edition, Addison Wesley Publ. Co. 1993

3. F. A. Cotton, G. Wilkinson and P.L. Gaus, "Basic Inorganic Chemistry", 3rd Ed., John Wiley 1995.

4. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, "Advanced Inorganic Chemistry" 6th Ed. John Wiley (Asia)

5. J. D. Lee, “Concise Inorganic Chemistry”, 5th ed. Chapman and Hall, 1996.
6. N. N. Greenwood and A. Earnshaw, “Chemistry of the Elements” Pergamon Press, Exeter, Great Britain 1984.
7. S. J. Lipard and J.M. Berg, “Principles of Bioinorganic chemistry”, Panim Publising Corporation, New Delhi 1997.
8. D. T. Sawyer, A. Sobkowak, J. L. Roberts Jr., “Electrochemistry for chemists”, 2nd Ed. John Wiley, Inc., New York, 91995.
9. A. G. Sykes, “Advances in Inorganic Chemistry” Academic Press Ltd, UK Ed, 1991.

CHIO – 505 LABORATORY COURSE IN INORGANIC CHEMISTRY – I

(4 Credit)

Group – 1: Group – 1: Preparation Inorganic compounds/ coordination compounds and estimations of metals: (30)

1) Preparation of acetylacetonate complexes of Co(II) and Co(III) and estimation of cobalt
2) Preparation of oxalate complexes of Fe(II) and Fe(III) and estimation of iron
3) Preparation of aluminiium(III)tris(acetylacetonate) and estimation of aluminium
4) Preparation of potassium dihydroxodioxalatotitanate(IV) and estimation of titanium
5) Preparation of $K_2ON(SO_3)_2$ (Fremy's salt)

Note: Wherever possible IR and other spectral studies should be undertaken

Group – 2: General experiments (35)

1) Analysis of soda ash by acidimetry
2) Analysis of talcum powder for Mg by complexometric titration
3) Analysis of Fe in pharmaceutical preparation (colorimetrically)
4) Analysis of borax (titrimetry)
5) Determination of the strength of commercial phosphoric acid by pH titration
6) Percentage purity of ZnO complexometric titration
7) Percentage purity of Epsum Salt by complexometric titration
8) Crystal growth experiments

Group – 3: Ore / Alloy/ commercial sample analysis (35)

1) Analysis of Goan Iron ore Ferro-manganese: a) Percentage moisture, b) Acid insoluble residue, c) Iron gravimetrically / Mn gravimetrically
2) Analysis of Bauxite: a) Aluminum gravimetrically
3) Analysis of Ilmenite ore
4) Analysis of Magnesite ore
5) Analysis of lime stone a) loss on ignition b) estimation of calcium (redox titration) c) calcium and magnesium by complexometrically
6) Analysis of sea shell for calcium content
7) Analysis of wood's metal
8) Analysis of leaded bronze, gun metal
9) Analysis of Brass
10) Analysis of Steel, Ni in nickel steel gravimetrically
11) Analysis of monel metal Cu gravimetrically, Ni spetrophotometrically
12) Analysis of magnalium a) Mg – volumetrically or b) Al – gravimetrically
13) Analysis of bronze

Reference Books:

1. G. Brauer "Handbook of Preparative Inorganic chemistry" 2nd ed., Vol. 1 and 2, Academic Press New York 1967.

2. J. Bassett, R.C. Denny, G. H. Jeffery and J. Mandham, “Vogel’s Text Book of Quantitative Inorganic Analysis” 4^{th} ed. ELBS 1985.
3. G. Marr and B. W. Rockett, “Practical Inorganic Chemistry”, Van Nostrnad Reinhold London 1972.
4. G. Pass and H. Sutcliffe, “Practical Inorganic Chemistry” 2^{nd} Ed. Chapman and Hall 1985.
5. J. D. Woolins, “Inorganic Experiments” Wiley – VCH Verlag GmbH and Co, 2003

CHIO – 506 LABORATORY COURSE IN INORGANIC CHEMISTRY – II

(4 Credit)

Group – 1: Preparation of ligands (including distillation/ recrystallisation) /complexes/ inorganic compounds (30)

1) Preparation of Schiff Base - 1
2) Preparation of Schiff Base - 2
3) Preparation of substituted benizoic acids
4) Oxidation of p-Xylene
5) Preparation of manganic acetate and estimation of Mn
6) Preparation of chromium(II)acetate hydrate and estimation of Cr
7) Polyoxometallate syntheses

Note: Wherever possible IR and other spectral studies should be undertaken

Group – 2: Syntheses and characterization of materials (25)

1) Preparation of Perovskite oxides by precursor method 2) Estimation of metals in precursors and oxides, 3) Characterization of precursors by thermal analysis 4) Characterization of precursors and oxides by chemical analysis 5) X-ray diffraction studies of oxides

Electrical characterization: 6) direct current resistance: Two probe / Four Probe; 7) Dielectric behavior (BaTiO3)

Group–3: Instrumental experiments/separation of meal ions by ion exchange resins (25)

1) Determination of stability constant of complex ions in solution
a) Fe(III)-sulfosalicyalic acid
2) UV-visible spectroscopy of transition metal complexes

Potentiometric determination of 3) cobalt 4) Nickel and 5) Zinc by EDTA 6) mixture of chloride and iodide

7) Conductance measurements: preparation and electrical conductivity measurements of some cobalt complexes
8) Determination of magnetic susceptibility of Mn(II), Cu(II) etc salts/complexes
9) Colorimetric estimation of urea, Hg, Cd
10) Separation of transition metal cations by cation – exchange chromatography
11) IR/NMR spectral studies of Inorganic compounds
12) Cyclic voltammetry experiment

Group – 4: Ore analysis/ Alloy analysis / analysis of commercial sample (15)

1) Analysis of pyrolusite
2) Analysis of Nickel-aluminium alloy

Group – 5: Semimicro analysis experiments (15)

1) Semimicro analysis (7 radicals including one rare earth) (cations and anions)

Reference Books:

1. G. Brauer "Handbook of Preparative Inorganic chemistry" 2nd ed., Vol. 1 and 2, Academic Press New York 1967.
2. J. Bassett, R.C. Denny, G. H. Jeffery and J. Mandham, "Vogel's Text Book of Quantitative Inorganic Analysis" 4th ed. ELBS 1985.
3. G. Marr and B. W. Rockett, "Practical Inorganic Chemistry", Van Nostrnad Reinhold London 1972.
4. G. Pass and H. Sutcliffe, "Practical Inorganic Chemistry" 2nd Ed. Chapman and Hall 1985.
5. J. D. Woolins, "Inorganic Experiments" Wiley – VCH Verlag GmbH and Co, 2003

M Sc-Part II Organic chemistry
Semester III and IV Courses

Compulsory courses			**Optional courses**		
Code	**Title**	**Credits**	**Code**	**Title**	Credits
CHOC 501	Organic Spectroscopy , Pericyclic Reactions and Photochemistry	**4**	**CHOO 501**	Chemistry of Natural Products	**3**
CHOC 502	Reaction Mechanisms and Stereochemistry	**4**	**CHOO 502**	Chemistry of Natural and Synthetic Polymers	**4**
CHOC 503	Synthetic Methods in Organic Chemistry	**4**	**CHOO 503**	Heterocyclic and Organometallic Chemistry	**4**
CHOC 504	Selected Experiments in Organic Chemistry	**4**	**CHOO 504**	Introduction to Medicinal Chemistry	**4**
			CHOO 505	Pesticides, Environmental Pollution and Newer Methods of Pest Control	**3**
			CHOO 506	Green Chemistry: An Introductory Course	**4**
			CHOO 507	Laboratory Course in Organic Synthesis	**4**
			CHOO 508	Innovative Experiments in Organic Chemistry	**4**
			CHOO 509	Dissertation	**8**
			CHOO 510	Laboratory Course in Medicinal Chemistry	**2**
			CHOO 511	Green Chemistry Techniques in Organic Synthesis	**3**
			CHOO 512	Laboratory course on Green Chemistry Techniques in Organic Synthesis	**2**

CHOC-501 : Organic Spectroscopy, Pericyclic Reactions and Photochemistry. (**4 Credits**)

1. **Electronic spectroscopy :** (8)

Theory of electronic spectroscopy (revision of the basic concepts), Application of electronic spectroscopy in organic chemistry.; Woodward- Fieser rules for calculating l_{max} for: i) conjugates, dienes, trienes and polyenes ii) a,ß- unsaturated carbonyl compounds

2. **Infra-Red Spectroscopy : (8)**

Theory of IR spectroscopy (revision of the basic concepts ; Applications of IR spectroscopy in structural elucidation of organic compounds (various functional classes to be considered)

3. **NMR Spectroscopy (14)**

Principles of NMR, instrumentation, chemical shift- (revision of the basic concepts); Interpretation of PMR spectra. a) Coupling constants and AB, AMX and ABX spin systems. b) Nuclear Overhauser effect and its applications. c) shift reagents.
CMR spectroscopy a) Double resonance and decoupling b) chemical shifts in CMR C0 interpretation of CMR spectra of organic compounds

4. **Mass spectrometry (10)**

Fragmentation modes a) McLafferty rearrangement and retro-Diels-Alderfragmentation b) Mass spectra of compounds like alcohols, amines, carbonyl compounds, hydrocarbons, halogen compounds, nitro compounds and cyanides.

5. **Structure elucidation of organic compounds using Combination of spectral methods described above. (10)**

6. **Pericyclic Reactions (25)**

Theory of pericyclic reactions- a) Frontier Molecuclar Orbital (FMO) theory b) Transition state aromaitcity (Mobius-Huckel theory) concept c) Orbital correlation diagram method

Analysis of pericyclic reactions (including stereochemistry)
a) Cycloaddition reactions b) Elelctrocyclic reactions c) Sigmatropic rearrangements

Some synthetically useful reactions

a) 1,3-dipolar additions b) Somlet-Hauser rearrangement c) [3,3] Shifts; Claisen and Cope rearrangements and fluxional molecules, d) ene reaction

7. **Photochemistry** (**25)**

Principles of energy transfer, theoretical concepts in organic photochemistry w.r.t. cycloadditions, electrocyclic reactions etc., Some photochemical reactions of alkenes, dienes, carbonyl compounds, arenes like a) cis-trans isomerization b) Paterno-Buchi reactionc)

photochemistry of arenes d) Barton reaction, Hoffman-Loffeler reaction e) Di-pi-methane rearrangement f) photochemical oxygenations g) Synthesis of theoretically interesting molecules like cubane, bullavalene

Reference Books :

1. Orbital Symmetry, R E Lehr and A P Marchand
2. Conservation of Orbital Symmetry, R B Woodward and R Hoffmann, Verlag chemie, Academic Press, NY, 1972.
3. Frontier Orbital Theory, I Fleming, Wiley
4. Pericyclic Reactions, , T L Gilchrist and R C Storr, Cambridge Univ. Press, 1972.
5. Advanced Organic Chemistry-Part A and B, F A Carrey and R J Sundberg, Pelnum Pub., 3rd Ed., 1990
6. Mechanisms and Thory in oragnic Chemistry T Lowery and K Richardson, Harper and Row Pub., NY, 3rd Ed., 1987.
7. Organic Photochemistry, Coxon and Halton, Cambridge Univ. Press, 1974.
8. Modern Molecular photochemistry, N Turro, Benjamin
9. Molecular Reactions and Photochemistry C H DePay, Prentice Hall (I) Ltd, New Delhi.
10. Organic Photochemistry- A Visual Approach, J Kopecky, VCH Pub., 1992.
11. Basic Principles of Organic Chemistry, Roberts and Caserio,W A Benjamin Inc., 2nd Ed., 1977.

Organic Spectroscopy

Text books:

1. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. and Wiley Eastern Ltd., Second edition, 1995.
2. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.

Reference books :

1. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
2. Absorption spectroscopy of organic Molecules, V.M. Parikh.
3. Spectroscopic methods in organic chemistry, Williams andFleming, Tata McGraw Hill ed., 1988, 4th ed.
4. Organic spectroscopy, William Kemp, ELBS, 2nd ed., 1987.

CHOC-502: Reaction Mechanisms and Stereochemistry (4 credit)

I Reaction Mechanisms

1. Hydrolysis/esterification of carboxylic esters/acids (5)

1.1 Classification and IUPAC nomenclature of the eight mechanisms for hydrolysis and formation of esters.

1.2 Mechanisms of acid and base-catalyzed hydrolysis and formation of esters with suitable examples.

2 The Neighboring Group Participation Mechanism and Anchimeric assistance (8)

2.1 General approach to the mechanism of the formation of NGP product and rearranged product.

2.2 Neighboring Group Participation by Unshared/lone pair of electrons

2.3 NGP by π-electrons

2.4 NGP by aromatic rings, (formation of phenonium ion intrmediate)

2.5 NGP by Sigma bonds with special reference to bornyl and *nor*-bornyl system (formation of non-classical carbocation)

3 Free radicals (17)

3.1 Introduction

3.2 Stability and structure of persistent and stable free radicals.

3.3 Detection of free radicals by magnetic susceptibility, spin trapping, esr and CIDNP methods.

3.4 Generation and fate of free radicals by (1)Thermal cleavage

(2) Photochemical cleavage (3) Electron transfer process

3.5 Different types of free radical reactions like

(1) Radical combination (2) Radical abstraction (displacement)

(3) Radical addition of multiple bonds (4) Radical addition to multiple bonds

(5) Fragmentation (β-elimination) (6) Rearrangements

(7) Disproportionation

3.6 Polar effects in radical reactions

3.7 Applications of radicals reactions in modern organic synthesis

(1) Formation Carbon halogen bonds: Substitution in saturated compounds, substitution in allylic and benzylic compounds, addition to C-C double and triple bonds, bromodecarboxylation (Hunsdiecker reaction). Iodo decarboxylation

(2) Formation of C-C bonds: Intra and intermolecularIntramolecular radical addition to C=C double bonds, polymerization of alkenes, Homolytic aromatic substitution, dimerization of alkyl radicals: Kolbe's electrolytic reaction, dimerization of aryl radicals Ullmann reaction

Coupling of alkynes, Acyloin synthesis

(3) Formation of C-N bonds

Nitrogen at saturated carbon , addition to C-C double and triple bonds, Hofmann-Loffler-Freytag reaction, Barton reaction

(4) Formation of C-O bonds
(5) Functional group transformations

4 Molecular rearrangements and their synthetic applications (20)

4.1 Unifying principles and mechanisms of rearrangements taking place at an electron deficient and electron rich substrates.

4.2 Rearrangements taking place at electron deficient carbon

(1) Arndt Eistert synthesis (2) Wagner Meerwein
(3) Benzil-benzilic acid (4)) Pinacol (5) Dienone phenol

4.3 Rearrangements at electron deficient nitrogen

(1) Hofmann (2) Curtius (3) Lossen (4) Schmidt (5) Beckmann

4.4 Rearrangements at electron deficient oxygen

(1) Baeyer Villiger (2) Dakin's reaction

4.5 Rearrangements at electron rich carbon

(1) Wittig (2) Favorskii (3) Stevens

4.6 Aromatic rearrangements

(1) Benzidine (2) Fries (3) Von Richter (4) Sommelet-Hauser

II Stereochemistry

1 Conformations, stability and reactivity of fused ring compounds (16)

1.1 Fused bicyclic systems with small and medium rings:

(1) Bicyclo [4.4.0] decanes (*cis*- and *trans*-decalins)
(2) *cis*- and *trans*-Decalones and decalols
(3) Octahydronaphthalins (octalins)
(4) Bicyclo [4.3.0] nonane (*cis*- and *trans*-hydrindanes)

1.2 Fused polycyclic systems

(1) Perhydrophenanthrenes
(2) Perhydroanthracenes
(3) Perhydrocyclopentenophenanthrene system (steroids, triterpenoids and hormones). Conformations and reactivity towards esterification, hydrolysis, chromium trioxide oxidation, ionic additions (of X_2) to double bonds, formation and opening of epoxide ring, epoxidation by peroxy acids.

2 **Conformation of bridged ring compounds (5)**

2.1 Bicyclo [2.2.1] heptane (norbornane)

(1) Geometry and topic relationship of hydrogens.
(2) Solvolysis of bicyclo[2.2.1]heptyl systems, formation, stability and reactivity of norbornyl cation.
(3) Relative stability and the rate of formation of endo and exo isomers in both bornane and norbornane systemes.

2.2 Bicyclo [2.2.2] octane system

(1) Geometry and topic relationship of hydrogens
(2) Solvolysis of bicyclo[2.2.2]octyl system.

2.3 Other bridged ring systems: starting from bcyclo[1.1.1]pentane to bicyclo[3.3.3] undecane

2.4 Bicyclosystem with heteroatoms: the relative stabilities of tropine, pseudotropine and benzoyl derivatives of norpseudotropine.

3 **Dynamic Stereochemistry: Stereoselective Reactions** **(13)**

3.1 Stereoselectivity: classification, terminology and principle.

3.2 Asymmetric synthesis and asymmetric induction with suitable examples.

3.3 Double diastereoselection and double asymmetric induction with suitable examples.

3.4 Strategy of stereoselective synthesis, acyclic stereoselection, addition of nucleophiles to carbonyl compounds, Cram's open chain and cyclic models

3.4 Enantioselective synthesis with suitable examples.

4 **Stereoisomerism due to axial chirality, planar chirality and helicity**. (**6)**

4.1 Stereochemistry and configurational (*R/S*) nomenclature in appropriately substituted allenes, alkylidene cycloalkenes, spiranes, adamantoids, biaryls, *trans*-cycloalkenes, cyclphanes and ansa compounds.

4.2 Atropisomerism in biphenyls and bridged biphenyls.

5 **Molecular dissymmetry and chiroptical properties** **(10)**

5.1 Circular birefringence and circular dichroism

5.1 ORD and CD curves: Cotton effect

5.3 Applications of CD and ORD

5.4 The octant rule and its applications to determine, configuration, conformation and structure.

5.5 The axial α-haloketone rule and its applications.

TEXT BOOKS :

1. Advanced Organic chemistry, reactions mechanism and structure by Jerry March Mc-Graw Hill Int. Book Co.
2. Stereochemistry of Organic compounds, Principles and applications by D. Nasipuri, 2nd edn. 1994 New Age International Pvt. Ltd.
3. Stereochemistry of carbon compound by E.L. Eliel, Tata, Mc-Graw Hill 1975.

REFERENCE BOOKS :

1. Stereochemistry and chemistry of Natural products by I.L. Finar, ELBS, Longman Edn.
2. Mechanism and structure in Organic chemistry by E.S. Gould, Holt, Rinehart and Winston.
3. Advance organic chemistry by F.A. Carey and R.J. Sundberg, Plenum Press.

Priciples of Organic Syntheses by R. O. C. Norman and Coxon, CRC Press Inc

CHOC-503 Synthetic Methods in Organic Chemistry (4 credit)

1. **Formation and reactions of enols and enolates.** (35)

1.1. Keto-enol tautomerism: introduction, acidity, basicity concepts and pKa scale, neutral nitrogen and oxygen bases. Formation of enols by proton transfer, requirements for and mechanism of enolisation catalysed by acids and bases, types of enols and enolates, kinetically and thermodynamically stable enols, consequences of enolisation, stable enolate equivalents, preparation and reactions of enol ethers.

1.2. Formation of Enolates: Introduction. preparation and properties, non-nucleophilic bases, *E* / *Z* geometry in enolate formation, kinetic *vs.* thermodynamic control, other methods for the generation of enolates, issue of enolate ambidoselectivity.

1.3. Alkylation of enolates: diverse reactivity of carbonyl groups, alkylation involving nitriles and nitroalkanes, choice of electrophile for alkylation, lithium enolates of carbonyl compounds and alkylation, specific enol equivalents to alkylate aldehydes and ketones, alkylation of □-dicarbonyl compounds, problem of regioselectivity during ketone alkylation and the remedy provided by enones.

1.4. Reaction of enolates with aldehydes and ketones: introduction, the aldol reaction including cross and intramolecular version, enolizable substrates which are not electrophilic in nature, controlling aldol reactions with specific enol equivalents, specific enol equivalents for carboxylic acids, aldehydes and for ketones.

1.5. Acylation at carbon: Introduction, the Claisen ester condensation (intramolecular and inter / crossed), acylation of enolates by esters, preparation of keto-esters by the Claisen reaction, directed C-acylation of enols and enolates and acylation of enamines.

1.6. Conjugate addition of enolates: Introduction, thermodynamic control *vs.* conjugate addition, utility of various electrophilic alkenes in conjugate addition, formation of six-membered rings *via* conjugate addition and nitroalkanes as versatile synthons.

1.7. Examples pertaining to the Application of following Condensation Reactions in Organic Synthesis : The Mukaiyama Reaction, Perkin Reaction, Dieckmann Condensaton, Knoevenagel Condensation and Doebner modification. The Stobbe Condensation, Darzens Glycidic Ester Condensation, Michael Addition, Robinson Annulation and selectivity and the Sakurai Reaction.

(10)

2. **Synthetic utility of the following name reactions / methodology with specific examples :** The Mannich Reaction, Hofmann - Loffler - Freytag Reaction, The Nef Reaction, The Mitsunobu Reaction, Intramolecular Fridel Crafts Cyclization Reaction. The Olefin Metathesis.

3. **The Ylids in Organic Synthesis.** (10)

3.1. Phosphorus Ylids: Nomenclature and Preparation. Wittig olefination: mechanism, stereoselctivity, *cis* and *trans* selective reactions, Wittig reagents derived from □-halo carbonyl compounds, Horner – Wadsworth – Emons modification with achiral and chiral substrates.

3.2. Controlling the geometry of double bonds: Peterson reaction and the Julia Olifination.

3.3. Sulfur Ylids: sulfonium and sulfoxonium ylids in synthesis, diphenylcyclopropyl sulfonium ylids and their reactions with carbonyl compounds / Michael acceptors.

3.4. Nitrogen Ylids: Formation, the synthetic utility of Stevens and the Sommelet rearrangement.

4. **Stereoselective / Asymmetric Synthesis.** (22)

4.1. General concepts of stereoselective and asymmetric synthesis. Selectivity in chemistry – substrate and product selectivity.

4.2. Stereoselective reaction of cyclic compounds: Introduction, reactions of four, five and six-membered rings. Conformational control in the formation of six-membered ring.

4.3. Diastereoselectivity: Introduction, making single diastereoisomers using stereospecific reactions of alkenes.

4.4. The diastereoselctivity in addition reaction to acyclic carbonyl compounds with □-chiral centre, rationalization of observed diastereoselctivity by using Felkin-Anh model, the effect of electronegative atom and chelation on stereoselctivity.

4.5. Stereoselctive reaction of acyclic alkenes: the Houk model, stereoselctive epoxidation, enolate alkylation. Diastereoselctivity in aldol reaction and stereoselctive ester aldols.

4.6. Asymmetric synthesis: Introduction, the chiral pool-Nature's "ready made" chiral centres, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions. Chiral auxiliaries - oxazolidinone and norephedrine-derived chiral auxiliary controlled Diels-Alder reaction and alkylation of chiral enolates, determination of enantiomeric and diastereomeric excess; enantio-discrimination relationship between optical rotation and optical purity. Resolution – optical and kinetic.

4.7. Enantiomeric separation: use of chiral column. Separating enantiomers spectroscopically: Moscher's ester method and chiral shift reagents. Chiral reagents and chiral catalysts: preparation and use of CBS asymmetric reducing agent, bakers yeast reduction, asymmetric hydrogenation using BINAP-Ru (II), DIPAMP-Rh complexes. Sharpless asymmetric epoxidation / dihydroxylation reaction: enantioselectivity and mechanism, synthesis of propranolol / chloramphenicol.

5. **Retrosynthetic (antithetic) Analysis.** (12)

5.1. Introduction, the disconnection protocol, guidelines for choosing a good disconnection, functional group interconversions (FGI), synthetic problems where the starting material is provided. Consecutive *vs. c*onvergent Syntheses.

5.2. Antithesis of simple achiral and chiral open – chain target molecules (1, 2 to 1, 6-difunctional), mono, bicyclic and bridged polycyclic molecules.

6. **Protecting Groups in Organic Synthesis.** (11)

6.1. Introduction, when are Protecting Groups needed? effective use of protective groups. Umpolung of reactivity and protecting groups.

6.2. Common protective groups namely acetals and ketals, ditho acetal/ketals, trialkylsilyl, TBDMS, THP, -OMPM, MOM, MTM, MEM, SEM and benzyl ether, methyl ether,

benzyl amine, Cbz, t-Boc, Fmoc, *t*-butyl ester and methods for deprotection. Examples of multistep synthesis using protection-deprotection procedures.

Reference Books

1. Advanced Organic Chemistry – Reaction Mechanisms, R. Bruckner, Harcourt / Academic Press, San Diego, 2002.
2. Organic Synthesis, M. B. Smith, McGraw – HILL International Edition, New York, 1994.
3. Some Modern Methods of Organic Synthesis, W. Caruthers, Cambridge University Press, New Delhi, 2003.
4. Organic Synthesis – Concepts, Methods, Starting Materials, J. Fuhrhop and G. Penxlin, VCH Publishers, Inc., New York, 1994.
5. Stereoselective Synthesis, M. Nogradi, VCH publishers, Inc., New York, 1994.
6. Modern Synthetic Reactions, H. O. House, W. A. Benjamin, New York.

Named Organic Reactions, T. Laue and A. Plagens, John Wiley, 2005

CHOC -504 : Selected Experiments in Organic Chemistry (4 credit)

1. Organic mixture separation (65)

Three component mixture separation based upon differences in the physical and the chemical properties of the components. elemental and functional group analysis and determination of physical constants of the individual compounds.
(Identification of the components is not expected).
(Minimum 13 experiments of 6hrs each.)

2. Organic Preparations (35)

Organic preparations based upon the reactions studied in the theory courses
(Minimum 7 experiments; Multi-step synthesis is to be emphasized).

Text Books :

1.Systematic qualitative organic analysis by H. Middleton, Tata McGraw Hill Publication
2.Advanced Practical Organic Chemistry by N.K. Vishnoi

Reference books:

1.Practical organic chemistry including qualitative organic analysis by A.I Vogel, 4th Edn ELBS, Longman.
2.Fundamentals of preparation organic chemistry by R.Keese. R.K.Muller and T.P Toube
3.Practical organic chemistry, F G Mann and B C Saunders,Orient Longman, 4th ed.
4.Elementary practical organic chemistry- part III, Quantita¬tive Organic analysis, A I Vogel,CBS Publishers, N Delhi.
5.Elementary Practical Organic Chemistry, Part II : Qualitative Organic Analysis, by A.I.Vogel, ELBS, Longman.

CHOO-01: Chemistry of Natural Products (3 credit)

1. **Source and isolation of Natural Products. (5)**

1.1 General methods of isolation

The modern distillation process, maceration, enfleurage, extraction by cold pressing and extraction with solvents,

2. **General methods of purification and structure elucidation of Natural Products (9)**

2.1 Fractionation of the crude extracts and purification of the individual compounds from the respective fractions using chemical and chromatographic techniques such as Column Chromatography, TLC, Preparative TLC, HPLC, etc.

2.2 Chemical methods based on the functional groups present. Bicarbonate extraction, sodium bisulphite adduct formation, derivatization, etc.

2.3 General approach to structure elucidation of the isolated pure compounds using UV, IR, NMR spectroscopy, MS spectrometry, optical polarimetry.

3. **Structure elucidation by classical chemical methods (14)**

3.1 Terpenoids: α-cedrene

3.2 Alkaloids: Morphine, thebaine and codeine

3.3 Steroids: Cholesterol, bile acids

4. **Structure elucidation by combination of chemical and spectral methods (13)**

4.1 Terpenoids: α- and β-vetivones, Ishwarone

4.2 Hormones: Cecropia Juvenile hormone, brevicomin and frontalin

4.3 Oxygen heterocycles: Aflatoxin-B1, rotenone

5. **Structure elucidation involving stereochemistry, spectral and Chemical methods (11)**

5.1 Terpenoids: Menthol and hardwickiic acid

5.2 Alkaloids: Reserpene

6. **Synthesis of selected Natural Products, planning and execution (26)**

5.1 Terpenoids: Longifolene (E J Corey), Caryophyllene (E J Corey) Nootkatone (A Yoshikoshi), Menthol (Tagasago)

5.2 Alkaloids: Reserpine (R B Woodward), Morphine (Marshall Gates)

5.3 Hormones: Cecropia JH (Edward), Progesterone

5.4 Prostaglandins: Prostaglandin E_2 (E J Corey)

5.5 Antibiotics: Cephalosporin (R B Woodward)

7. **Biogenesis and biosynthesis of Natural Products (22)**

7.1 Terpenoids and Steroids: General approach towards biosynthesis of mono-, sesqui-, di-, tri-, tetraterpenoids and steroids through mevalonate pathway with special reference to the biosynthesis of terpenoids and steroids included in topics 3 to 6

7.2 Alkaloids: The shikimate pathway formation of hydroxybenzoic acid derivatives, aromatic amino acids, L-phenylalanine, L-tyrosine, phenolic oxidative coupling, biosynthesis of thebaine, codeine and morphine,

References for Theory

1. Organic Chemistry: Stereochemistry and the Chemistry of Natural Products, Finar, I L, ELBS edition.
2. Natural Product Chemistry by Koji Nakanishi, Academic Press.
3. The Alkaloids by D. R. Dalton, Marcel Decker.
4. Comprehensive Organic Chemistry by Barton and Olis.
5. Medicinal Natural Products, a Biosynthetic Approach, Derick Paul, John Wiley and Sons, 2002.
6. Biosynthesis of Natural Products, Mannitto Paolo.
7. Selected Organic synthesis by Ian Fleming, John Wiley and Sons
8. Total synthesis of Natural Products, J. ApSimon, John Wiley and Sons.
9. The Logic of Chemical Synthesis , E. J. Corey and Xue-Min Cheng, Wiley Interscience, a division of John Wiley and Sons Inc.
10. Classics in Total Synthesis , K. C. Nicolaou and E. J. Sorensen, Weinhem: VCH, 1996

CHOO-502: Chemistry of Natural and Synthetic Polymers (**4 Credits)**

1. Brief history of natural and synthetic polymers, **10**
Classification of polymers, Functionality concept- linear, branched and cross-linked polymers. Introduction to biodegradable polymers

2. **Methods of polymerization** **10**
Bulk, solution, suspension, emulsion, addition, condensation polymerizations.
Ionic and co-ordination polymerization reactions and copolymerization.

3. **Some properties of polymers** **10**
Number and weight average molecular weights, Molecular weight distribution, polydispersity, Glassy state and glass transition temperature, crystallinity in polymers. Introduction to characterization of polymers

4. **Additives in polymers** **15**
Lubricants, plasticizers, stabilizers, antioxidant, fillers etc., (properties and examples)

5. **Resources for monomers, manufacture of some important monomers and reagents viz.,** **20**
Ethylene, propylene, butadiene, isoprene, styrene, divinyl benzene, acrylates, acrylonitrile, vinyl chloride, formaldehyde, adipic acid, urea, bisphenol-A, melamine, terephthalic acid, phthalic anhydride, dimethyl terephthalate, glycol, glycerol, ethylene oxide, epichlorohydrin, capro-lactum, di-isocyanates, pentaerythritol.

6. **Synthesis, properties and applications of-** **20**
Vinyl polymers- LDPE, HDPE, PVC, PVA, polyvinyl acetate, polyacrylates, methacrylates, polystyrene, teflon, ABS, SBR, SAN.
Condensation polymers- Nylons, polyesters, polyurethanes, polycarbonates.
Cellulose esters- cellulose acetate, nitrates and acetate-butyrates.
Natural rubber, Thermoset resins- phenol-formaldehyde, resols and novolacs, melamine-formaldehyde, urea-formaldehyde, epoxy resins - their curing.

7 Polymer processing – Introduction to compounding, and processing techniques like calendaring, casting, moulding and spinning in polymer processing. **15**

Text Books:

1 Polymer science- V R Gowarikar and others; Wiley Eastern Ltd., 1986.
2. Principles of Polymer science- P Bahadur and N V Sastry, Narosa Publishing House, 2003.
3. Polymer Science and Technology- J R Fried, PHI Pvt Ltd., 2000
4. Outlines of Polymer Technology- R Sinha, PHI Pvt Ltd.,
   i. Manufacture of Polymers- 2000
   ii. Processing Polymers- 2003

Reference Books :

1. Plastic Materials- J A Brydson; Newnes-Butterworths 3rd Ed. 1979, p.73.
2. Handbook of analysis of synthetic polymers and plastics- J Urbansky and others; John Wiley, 1977 .
3. Organic polymer chemistry- K Y Saunders; Chapman and Hall, UK, 1976.
4. Organic chemistry of synthetic high polymers- R W Lenz; 1967.
5. Handbook of polymer synthesis- Kircheldorf H R (Ed); Marcel Dekkar Inc., 1992, PART A and B
6. Handbook of plastic test methods- Brown R P; 2nd ED, George Godwin Ltd., 1981.
7. Polymer Chemistry- An Introduction- M P Stevens; 2nd Ed, Oxford Univ. Press, 1990.
8. New methods in polymer synthesis- W Y Mijs (Ed); Pelnum Press Ltd., NY, 1992.
9. Polymer chemistry- the basic concepts- P C Hiemenz; Marcell Dekkar Inc., 1984.
10. Industrial chemicals- W L Paith, D B Keyes ad R L Clark; John Wiley and Sons.
11. Introduction to polymer chemistry- W R Moore; Univ. of London Press.
12. Handbook of polymer science and technology- N P Cheremisinoff (Ed), Volumes 1-4, 1989.
13. Comprehensive polymer science- Synthesis, characterization, reactions and applications of polymers; Volumes 1-7, Pergamon Press, NY, 1989.

CHOO-503: Heterocyclic and Organometallic Chemistry (4 credit)

1. Introduction, classification and Nomenclature of mono and bicyclic heteroaromatic molecules (**5**)

2. Physical properties, dipole moment, acidity-basicity, Aromaticity electron density distribution and reactivity of- **(25)**
2.1 Furan, Thiophene,Pyrrole, Indole
2.2 Pyridine, Pyridine-N-oxide
2.3 Quinoline and isoquinoline

3. Synthetic strategies based on reterosynthetic approach General methods of synthesis of the following- **(20)**
3.1 Furan, Thiophene, Pyrrole, Indole
3.2 Pyridine, Quinoline and isoquinoline

4. Introduction to organometallic chemistry: (**10**)
4.1 Metal-carbon bonds with main-group metals and transition metals:
4.2 Sigma and pI bonds
4.3 Nomenclature and heptacity
4.4 Electron counting and 18e rule
4.5 Orbital interactions and bonding
4.6 Kinetic stability.

5. Organomatallic compounds Main group elements (**20**)
Preparation, properties and applications of lithium Magnesium, Cadmium, Zinc, Cerium, Murcury and Chromium compounds

6. Transition metals in organic synthesis **(20)**
Preparation, properties and applications of Copper, Palladium and Nickel reagents..

REFERENCE BOOKS:

1. Heterocyclic Chemistry, J A Joule and G F Smith, ELBS,
2. Heterocyclic Chemistry, John A. Joule and Keith Mills
2. Heterocyclic Chemistry, T L Gilchrist, Pitman, 1985
3. An Introduction to Chemistry of Hetreocyclic Compounds, R M Acheson,John Wiley and Sons 3rd Ed., 1977.
4. Heterocyclic Chemistry, D W Young, Longman Group Ltd., London, 1975.
5. Principles of Heterocyclic Chemistry, A R Katritzky and J M Lagowskii, Mathesons and Co., 1967.

6. Chemistry of Heterocyclic Compounds, Edited by A Weissberger and E Taylor, Vol. 1 to 47, 1987.
7. Advances in Heterocyclic Chemistry, Edited by A R Katritzky etal,Vol. 1 to 50, Academic Press

REFERENCE BOOKS:

1. Comprehensive Organometallic Chemistry, 2nd Edition, 14 vols. Pergman, 1995.
2. Chemistry of Metal-Carbon Bond, 6 vols. (Ed). F.R. Hartley, Wiley 1982-83.
3. Advanced Organic Chemistry,F A Carey and R Sundberg, Vol. B, Plenum Press (old and new editions)
4. Organometallics in Synthesis - A Manual (Ed.) M. Schlosser, John, Wiley, 1994.
5. The Organometallic Chemistry of the Transition Metals, R.H. CraJohn Wiley, 1994.
6. Transition Metal Organometallics for Organic Synthesisand G.R. Stephenson, Cambridge University Press, 1991.
7. Advances in Metal Organic Chemistry, Vols. 1 and 2 (Ed.) L.S. Liebeskind, JAI Press,1989.
8. Principles and Applications of Organotransition Metal Chemistry, J.P. Colliman, L.S.Hegedus, J.R. Norton and R.G. Finke, University Science Books, 1987.
9. Organotransition Metal Chemistry - Fundamental Concepts and Applications, A. Yamamoto, Wiley, 1986.
10. Metallo-Organic Chemistry, A.J. Pearson, John Wiley, 1985.

CHOO-504 Introduction to Medicinal Chemistry (4 credit)

1. Introduction to Drugs. (7)

1.1. Requirement of an ideal drug 1.2. Sources of drugs 1.3. Important terms used in chemistry of drugs 1.4. Classification and nomenclature of drugs 1.5. Drugs and the medicinal chemists.

2. Drug Design. (10)

2.1. Analogues and pro-drugs 2.2. Concept of lead compounds 2.3. Features governing drug design – The method of variation, drug design through disjunction, conjunction, tailoring of drugs 2.4. Cimetidine – a rational approach to drug design.

3. Drug Development. (10)

3.1. Screening of natural products, isolation and purification, structure determination 3.2. Structure-activity relationship, QSAR, Synthetic analogues 3.3. Natural Products as leads for new pharmaceuticals 3.4. Receptor theories 3.5. Oxaminiquine – a case study.

4. Mechanism of drug action. (10)

4.1. Introduction 4.2. Enzyme stimulation 4.3. Enzyme inhibition 4.4. Sulfonamides 4.5. Membrane-active drugs 4.6. Polymorphism and drug delivery.

5. Study of the following class including the synthesis of major drugs (30)

5.1. Pharmacodynamic Agents.

a) Local anesthetics b) Analgesics : narcotic and non-steroidal anti-inflamatory, narcotic antagonists c) Antiepileptic drugs d) Antiparkinsonism drugs e) Antihistaminics f) Seditives and hypnotics g) Antipsychotics

h) Cardiovascular agents : Cardiovascular diseases, Antianginal agents and vasodilators, Antihypertensive agents, Antiarrhythmic drugs, Adrenergic blocking agents

i) Antihyperlipidemic and antiatherosclerotic agents

j) Anticoagulants, blood coagulation and anticoagulant mechanism

k) Diuretics l) Drugs and diabetes : Synthetic hypoglycemic agents.

5.2. Chemotherapeutic Agents. (13)

a) Sulfonamides b) Antitubercular and Antilepral agents c) Antiamoebics d) Anthelmintics e) Antimalarials f) Antiviral agents g) Antineoplastic Agents

5.3. Antibiotics : General information, mode of action and application of: (13)

a) □-Lactam antibiotics : Penicillins and Cephalosporins

b) Aminoglycocides : Streptomycin, Neomycin c) Tetracyclines

d) Macrolides : Erythromycin, Rifamycin e) Lincomycin

f) Polypeptides : Bacitracin g) Unclassified antibiotics : Chloramphenicol

6. **New Developments and new problems. (7)**

6.1. Introduction 6.2. Gene therapy 6.3. Drug resistance 6.4. Antisense drugs 6.5. Cytokines 6.6. Drugs to combat AIDS.

Reference Books:

1. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 8th edition Edited by Robert F. Doerge, J. B. Lippincott Company, Philadelphia, USA
2. Burger's Medicinal Chemistry, Part I and II, 4th edition, Edited by M. E. Wolff, John Wiley.
3. Principles of Medicinal Chemistry, W. O. Foye, 3rd edition, K. M. Varghese and Co., Bombay.
4. Organic Chemistry of Drug Synthesis, Lednicer and Mitscher, Vols I and II, John Wiley.
5. An Introduction to Medicinal Chemistry, Graham Patrick, Oxford University Press, Oxford, 1998.
6. Burgers Medicinal Chemistry and Drug Discovery, Vol. I, 6th edition, Edited by Donald J. Abraham, John Wiley and Sons, New Jersey, 2003

CHOO-505 Pesticides, Environmental Pollution and Newer Methods of Pest Control

(3 credit)

1. **Introduction** (9)

1.1 The Shape of the Pesticide Industry

1.2 Pesticides in the Developing World

1.3 Defense Mechanisms in Plants

1.4 Types of Pests including house hold and stored grain and grain products

2. **Types of Pesticides** (9)

2.1 Classification

2.2 Toxicology and Mode of Action

2.3 Sanitary Fundamentals of Pesticide Application

(26)

3. **A) Important group of Pesticides** (method of preparation and uses of important pesticides in use under each group/sub-group is expected)

3.1 Insecticides

3.2 Fungicides

3.3 Weedicides and Herbicides

3.4 Rodenticides and Fumigants

3.5 Acaricides and molluscicides

3.6 Nematicides

B) Industrial Process for the manufacture of 2, 4 – D and Parathion with flow sheet diagram

4. **Behaviour Controlling Compounds** (7)

4.1 Attractants

4.2 Repellants

4.3 Chemosterilants

4.4 Antifeedants

4.5 Oviposition Inhibitors

5. **Naturally occurring Insecticides (Botanical Pesticides)** (6)

5.1 Pyrethroids

5.2 Rotenoids

5.3 Other insecticides of plant origin (Ryania, Neem, Nicotine etc.,)

6. **Synthetic Pyrethroids** (6)

6.1 Types of Compounds

6.2 Structure-Activity Relationship

6.3 Toxic Action and Synergism

6.4 Synthesis of important pyrethrins and their uses.

7. **Influence of Pesticides on Environment** (17)

7.1 Behaviour of Pesticides in the air, water and soil

7.2 Action of Pesticides on Biocoenoses, Birds and Animals

7.3 Bioaccumulation of Pesticides

7.4 Integrated System of Plant Protection-The basis for Preventing the harmful action of Pesticides on the environment

8. **Newer Methods of Pest Control** (20)

8.1 Use of Morphogenetic Agents (Hormones and Pheromones)

8.2 Microbial Pesticides

8.3 Chitin and Amino acid Synthesis Inhibitors

8.4 Sexual Sterilization and utilization of Behaviour Controlling Compounds

8.5 Future Trends in pest control

Reference Books:

1. Diseases in Plants – An Introduction to Agricultural Phytopathology by Neil E. Stevens and Russell B. Stevens.
2. Modern Toxicology, P. K Gupta and D. K. Salunki, Metropolitan Book Co., New Delhi.
3. Toxicology, Mechanism and Analytical Methods, C. P. Stewart and A. sholman, Academic Press N. Y. and London.
4. Ecology of Pesticides, A. W. A Brown, Wiley Interscience Pub.
5. Monograph on Neem (*Azadirachta indica A. Juss.*), D. N. Tewari, Indian Council of Forestry Research and Education, Dehradun, India.
6. Riegels Handbook of Industrial Chemistry, 8th edition, James A Kent, Van Nostrand Reinhold Comp.
7. Fungicides, Edited by Dewayne C. Torgeson, Vol. I, Academic Press.
8. Pesticides in the Environment, Vol. II and III, Edited by Robert White-Stevens, Marcel Dekker INC, N. York.
9. Chemicals for Crop Protection and Pest Control, M. B. Green, G. S. Hartley and T. F. West, Pergamon Press, Oxford.
10. Chemistry of Monoterpenes, William F. Erman, Marcel Dekker INC., New York.
11. Naturally Occurring Insecticides, Edited by Martin Jacobson and D. G. Crosby, Marcel Dekker INC., New York.
12. Herbicides : Chemistry, Degradation and Mode of Action, 2nd Edition, Vol. I and II, Edited by P. C. Kearney and D. D. Kaufman, Marcel Dekker INC., New York.
13. Insecticides of the Future, Edited by Martin Jacobson, Marcel Dekker INC., New York.
14. Chemistry of Pesticides, N. M. Melnikov, Residue Reviews, Vol., 26, Springer Verlag, New York.
15. Future for Insecticides, R. C. Metcalf and J. J. Mc. Kalvery, Jr. John Wiley and Sons, New York.
16. Pesticides Process Encyclopedia, Marshel Sitting Noyes Data Corporation, U. S. A.
17. Pesticides : Their Ecological Impact in Developing Countries, Edited by G. S. Dhaliwal and Balwinder Singh, Commonwealth Publishers, New Delhi, 1993.
18. The Chemical Protection of Plants, Edited by G. S. Gruzdyev, Mir Publishers, Moscow

CHOO-506 Green Chemistry: An Introductory Course (4 credit)

1. Principles and Concepts of Green Chemistry (10)

Introduction, twelve green principles, sustainable development and green chemistry.

Atom Economy: atom economic reactions- rearrangement and addition reactions.

Atom un-economic reactions- substitution, elimination and Wittig reactions.

Reducing toxicity.

2. Waste: Production, Problems and Prevention (13)

Introduction, Some problems caused by waste, sources of waste from the chemical industry and the cost of waste.

Waste minimization techniques: the team approach and process design for waste minimization, minimizing waste from existing processes.

On-site waste treatment: Physical, chemical and biotreatment.

Design for degradation: degradation and surfactants, DDT, polymers and some rules for degradation.

Polymer recycling: separation and sorting, incineration, mechanical recycling and chemical recycling to monomers.

3. Measuring and Controlling Environmental Performance (10)

3.1. The importance of measurement: Lactic acid production, safer gasoline.

3.2. Introduction to life cycle assessment and green process metrics.

3.3. Environmental management systems: ISO and European Eco-Management and Audit Scheme, eco-labels, green chemical supply Strategies, Legislation and integrated pollution prevention and control.

4. Catalysis and Green Chemistry (17)

4.1. Introduction to catalysis and comparison of catalyst types.

4.2. Heterogeneous catalysts: Basics of heterogeneous catalysis, Zeolites and the bulk chemical industry, heterogeneous catalysis in the fine chemical and pharmaceutical industries. Catalytic converters.

4.3. Homogeneous catalysis: Transition metal catalysts with phosphine ligands, greener Lewis acids and asymmetric catalysis.

4.4. Phase transfer catalysis: Hazard reduction, C – C bond formation and oxidation using hydrogen peroxide.

4.5. Biocatalysis and photocatalysis.

5. Organic Solvents: Environmentally Benign Solutions (13)

5.1. Organic solvents and volatile organic components, solvent free systems.

5.2. Supercritical fluids: supercritical carbon dioxide and supercritical water.

5.3. Water as a reaction solvent and water-based coatings.

5.4. Ionic liquids as catalysts and solvents.
5.5. Fluorous biphase solvents.

6. Renewable Resources (12)

Biomass as a renewable resource. Energy: Fossil fuels, biomass, solar power, fuel cells and other forms of renewable energy.

Chemicals and polymers from renewable feedstock.

Alternative economies: the syngas economy and the biorefinery.

7. Greener Technologies and Alternative Energy Sources (13)

Design for energy efficiency

Photochemical reactions: advantages of and challenges faced by photochemical processes,

examples of photochemical reactions.

Chemistry using Microwaves: microwave heating and microwave-assisted reactions.

Sonochemistry and green chemistry examples.

Electrochemical synthesis and examples.

8. Industrial case studies (12)

A brighter shade of green: synthesis of stilbene intermediates for optical brightners.

Greening of acetic acid manufacture, EPDM rubbers and Vitamin C.

Leather manufacture: tanning and fatliquoring.

Dyeing to be green: some manufacturing and products improvement and dye application.

Polyethene: Radical process, Ziegler – Natta and metallocene catalysis.

Eco-friendly pesticides.

Reference books

1. Green Chemistry, Mike Lancaster, The Royal Society of Chemistry, Cambridge, UK, 2002.
2. Green Chemistry: Environmentally Benign Reactions, V. K. Ahluwalia, Ane Books India, New Delhi, 2006.
3. Introduction to Green Chemistry, Albert S. Matlack, Marcel Dekker, Inc., New York, 2001.
4. Green Chemistry: Frontiers in benign chemical synthesis and processes, Paul T. Anastas and Tracy C. Williamson (Eds.), Oxford University Press, Oxford, 1998.
5. Green Chemistry: Environment Friendly Alternatives, Rashmi Sanghi and M. M. Srivastava (Eds.), Narosa Publishing House, New Delhi, 2007.
6. Green Chemistry, Samuel Delvin, IVY Publishing House, Delhi, 2006.
7. New Trends in Green Chemistry, V. K. Ahluwalia and M. Kidwai, Anamaya Publishers, N. Delhi, 2004.
8. Chemical Synthesis using Supercritical fluids, P. G. Jessop and W. Leitner (Eds.), Wiley – VCH, Verlag, Weinheim, 1999.
9. Solvent Free Organic Synthesis, Koichi Tanaka, Wiley – VCH GmbH and Co. KgaA, Weinheim, 2003.

10. Green Chemistry, Theory and Practice, P. T. Anastas and J. C. Warner, Oxford University Press, N. York, 1998.
11. Organic Reactions in aqueous Media, C - Jun Li and T – Hang Chan, John Wiley and Sons INC., N. York, 2001.
12. Organic Synthesis on Solid Phase, F. Z. Dorwald, Wiley – VCH Verlag, Weinheim, 2002.
13. Ionic Liquids in Synthesis, Peter Wasserscheid and Tom Welton (Eds.), Wiley – VCH Verlag, Weinheim, 2003.
14. Microwaves in Organic Synthesis, Andre Loupy (Ed.), Wiley – VCH Verlag, Weinheim, 2002.
15. High Pressure Chemistry, R. Van Eldik and F. G. Klarner (Eds.), Wiley – VCH Verlag, Weinheim, 2002

CHOO-507 : Laboratory course in Organic Synthesis 4 credits

It is mandatory that the concerned teacher sensitizes the students on the theoretical aspects/considerations of each experiment before asking the students to carry out the same. The students are required to undertake pre-lab. and post – lab. assignment as instructed by the concerned teacher and the same may be evaluated by according suitable weightage as an ISA component while prescribing the mode of assessment.

(Group A ; minimum 10 experiments)

1. Dimedone from mesityl oxide (Dieckmann condensation).
2. 1,2,3.4 - tetrahydrocarbazole from cyclohexanone (Fisher indolisation realtion).
3. Photochemical transformation of benzophenone to Benzopinacol.
4. 2 - (4-Methyl benzoyl) benzoic acid from pthalic anhydride and toluene (F.Cralis reaction).
5. 2 - (4-Methyl berrzoyl) benzoic acid to methyl anthraquinone (PPA cyclisation).
6. Resolution of racemic phenyl ethylamine using tartaric acid.
7. Trans - Stilbene by Wittig reaction.
8. Enamine alkylation :2- methyl cyclohexanone pyrrolidine enamine with CH3I.
9. o - Chlorobenzylidene rhodanine (Perkin reaction).
10. Diels - Alder reaction of anthracene and maleic anhydride using microwave irradiation.
11. Oxidation of a primary / secondary alcohol to carbonyl compound by polymer supported chromic acid (Amberlyst A - 26, chromate form).
12. Phenytoin from benzil and urea.
13. Use of protecting groups: Synthesis of I ,1- diphenyl- 1 -.butene - 3 - one

1) Ethyl acetoacetate ethy,lene acetal.
2) 1,1 - Diphenyl - 1 - hydroxy-3- butanone ethylene acetal.
3) 1,1 - Diphenyl - 1 - hydroxy - 3 - butanone.
4) 1,1 - Diphenyl - I - buten - 3 -one.

14. Isoborneol from camphor (NaBH4 reduction)
15. 3 -Methyl -2-phenyl-2-butanoI from 2-bromopropane and acetophenone
16. F. C. acylation of anisole

(GROUP B ; minimum 10 experiments)

l. Triphenyl carbinol from benzophenone or ethyl benzoate (Grignard reaction).
2. Benzidine from hydrazobenzene (benzidine rearrangr:ment).
3. Methyl orange/red from sulphanilic acid/anthranilic acid (diazotization).
4. Benzil to hydrobenzoin (NaBH4 reduction).
5. Epoxidation of cholesterol or related compounds
6. 2,2 - dichloro bicyclo (4.1.0) heptane from cyclohexene and dichloro cabene using PTC.
7. Reduction of Nitrobenzene to aniline by Sn / HCl.
8. 2 - methyl benzimidazole from o-phenylene diamine.

9. Benzophenone oxime to benzanilide (Beckmann rearrangement).
10. Ferric chloride oxidative coupling of 2-naphthol: 2,2'- dihydroxy dinaphthyl
11. Dicoumarol from coumarin derivative.
12. LAH reduction of Anthranilic acid.
13. Norborneol to norcarnphor using chromiurn trioxide/sulfuric acid
14. Halogenation using NBS: preparation of 9-bromoanthracene (or benzylic bromides)
15. Benzhydrol from benzaldehyde (Grignard reaction)
16. Ethyl n-butyl acetoacetate by acetoacetic ester condensation
17. Diethyl 4- butyl malonate by malonic ester condensation

Note: Students are expected to use techniques like TLC, FTIR, GC for monitoring/ establishing purity, identity of the synthesized compounds.

Reference books :

1. Experimental Organic Chemistry (2nd edition). H. Dupont Durest and Georg,-- 'W. rliol:e,I.Mc Grarv - I{ill Book tlompany, N. York. 1987.
2. Organic Chemistry Laboratory, O. R. Roding, C. E" Bell., Jr., A. K. Clark, Saunders College Publishing, Florida, 1990.
3. Chemistry Experiments for Instrumental Methods, D. T. Sarvyer, W. R. Heineman and J. M. Beebe, John Wiely and Sons, N. York, 1984.
4. Introduction to Organic Laboratory Techniques, D. L. Pavia, G. M" Lampman, G. S. Kriz and R. G. Engel, Saunders Sunburst Series, Saunders College Publishing, Philadelphia, 1995.
5. Microscale and miniscale laboratory experiments, A. M. Schoff Stall, B. A. (ja.jclis ancl M. L. Druelinger, Mc Graw - Hill Higher Education, 2000.
6. Macroscale and Microscale organic experiments, K. L. Williamson, D. C. Heath and Company, Levington, 1 989.
7. Organic Chemistry Experiments B. N. Campbell, Jr., M. M. Ali, Br66ks / C,cle Publishing Co. California, 1994.
8. Operational Organic Chemistry - A laboratory course (2ncl edition). J W. Lehman, Allyn and Bacon, [NC- Boston, 1988.
9. Microscale organic laboratory, D. W. Mayo, R. M. Pike and S. S. Btrtcher, John Wiley and Sons, N. York, 1989.
10. Solvent Free Organic Synthesis, Koichi Tanaka, WILEY - VCH GmbH and Co. KgaA. Weinheim, 2003.

CHOO-508 Innovative Experiments in Organic Chemistry 4 Credits

While Group 1 shall be compulsory, any other groups equivalent to 3 Credits are to be provided by the Department Council taking into account the theoretical background of the students opting for the course and availability of required instrumental facilities. *It is mandatory that the concerned teacher sensitizes the students on the theoretical aspects/considerations of each experiment before asking the students to carry out the same. The students are required to undertake pre-lab. and post – lab. assignment as instructed by the concerned teacher and the same may be evaluated by according suitable weightage as an ISA component while prescribing the mode of assessment.*

Group 1: Elucidation of structures of organic compounds using spectra (1 Credit)

UV, IR, PMR, CMR, Mass (Minimum 10 experiments of 3 hr duration each to be performed) . Depending upon available instrumental facilities, students be asked to record spectra of 2-3 unknown (UV, IR, PMR, CMR etc.) compounds/samples and the structure may be elucidated.

Note: *Spectral analysis assessment be conducted as follows : It is recommended that the candidate be given a combination of spectra (UV, IR, PMR, CMR, Mass) from which he will have to deduce preliminary information within first half an hour of the examination without referring to any book/reference material. (This shall carry not more than half of the maximum marks assigned to this exercise). The complete structure of the compound may then be elucidated by the candidate by referring to any standard text-book/reference material etc., (This shall carry remaining marks).*

Group 2: Ultrasound in synthesis (any 6 experiments, (1 credit)

a) Coupling reaction between a □□, □ – unsaturated carbonyl compound and acetone.
b) Aldol dimerisation of □□– tetralone catalysed by basic alumina.
c) 2-chloro-N-aryl anthranilic acid from 2-chlorobenzoic acid and 2-chloroaniline.
d) Butyraldehyde from 1-chlorobutane by the reaction of Li and dimethyl formamide.
e) One-pot synthesis of 3-nitro-2H-chromenes b1, the reaction of o-hydroxy benzaldehyde and nitro styrene by sonication.
f) Aldol dimerisalion of α-tetralone catalysed by basic alumina through sonication.
g) Cannizarro reaction of benzaldehyde under heterogeneous condition catalyzed by barium hydroxide and ultrasound

Group 3: Phase transfer catalysis (PTC) (any 5 experiments, (1 credit)

a) Darzens condensation of cyclohexanone with chloroacetonitrile to provide 1-oxaspiro-[2,5]-octane-2-carbonitrile.
b) *Syn* – hydroxylation of cyclooctene or cyclohexene with $KMnO_4$ solution.
c) Oxidation of benzyl alcohol with hypochlorite solution.
d) 3,4-diphenyl-7-hydroxycoumarin by the reaction of 2-hydroxy-4-methoxy benzophenone with phenylacetyl chloride.

e) Flavone from o-hydroxyacetophenone and benzoylchloride.
f) 2,2-dichlorobicyclo[4.1.0]heptane from cyclohexene and chloroform in presence of NaOH.
g) Toluene to benzoic acid by alkaline KMnO4.
h) Salicylaldehyde from phenol and chloroform.
i) 2-Benzoyl-3,5-dimethyl benzofuran from 2-hydroxy-5-methyl acetophenone and phenacyl bromide using pTC

Group 4: Microwave in organic synthesis (1 credit)

a. Esterfication of benzoic acid using microwave
b. Alkylation of ethyl acetoacetate using microwave conditions in presence of a PTC
c. Solvent free N-alkylltion of saccharin by microwave irradiation
d. Fries rearrangement of p-cresyl acetate by microwave irradiation
e. $KMnO_4$ oxidation of toluene assisted by microwave

Group 5: Photochemical reactions (1 credit)
a) Dimerization of cinnamic acid to truxillic acid.
b) Cyclisation of coumarin derivative in solid state / water.
c) Benzopinacol by reduction of benzophenone in isopropyl alcohol.
d) Isomerisation of trans-azobenzene to cis-azobenzene.
e) Photochemical isomerization of trans- azobenzene to cis-azobenzene-A TLC experiment
f) Photobromination of dibenzyl : Preparation of 1,2-dibromo-1,2-cliphenyl ethane
g) Photochemical reaction: Preparation of 9-hydroxy dixanthyl

Group 6: Polymer synthesis and characterization (2 Credits)

A) Polymer synthesis (any 4 experiments)
i. Phenol-formaldehyde resins- e.g. Bakelite
ii. Epoxy resins and their curing (e.g.Bisphenol-A and epichlorohydrin)
iii. Polyvinyls- polystyrene, e.g. PMMA, polyvinyal acaetate
iv. Condensation polymerization: e.g. Nylon 6-10 (polyhexamethylene sebacamide) from cebacoyl chloride and hexamethylene diamine

B) Qualitative Analysis of minimum three polymer samples.
HDPE, LDPE, PVC, PC, PMMA, PS, PET, alkyd resin

C) Quantitative analysis (minimum four experiments): To find--
SAP value, ester value, acid value, iodine value, epoxy value, amine value, OH value etc., of given polymer sample.

Group 7: Natural product chemistry (1 credit)
(any 6 experiments to be performed)

A Isolation of Natural Products

1. Microscale extraction of caffeine from tea, coffee, Coca-cola, etc. Purification of the caffeine extracted by microscale sublimation. Characterization by IR.
2. Isolation of cinnamaldehyde from cinnamon sticks by microscale steam distillation Characterization by IR

3 Microscale isolation and characterization of an optically active Natural Product Usnic acid from lichens. Characterization by IR

B Stereoselective enzymatic reduction

1 Enzymatic reduction of ethylacetoacetate using Baker's yeast
Purification of the chiral (+)-keto alcohol by distillation under reduced pressure.

2 Catalytic hydrogenation of an unsaturated Natural Product: e.g. (*R*)-Limonene, α-pinene, β-pinene, etc.

C Identification and separation of Natural Products

1 Thin Layer Chromatography of mixtures of Natural Products.

2 Column chromatography of a two component mixture of Natural Products

D Synthesis of Natural Products: Synthesis of camphor from camphne.

1 Conversion of Camphene to isobornyl 7 bornyl acetates

2 Hydrolysis of bornyl acetates to isoborneol and borneol

3 Oxidation of isoborneol and borneol to camphor.

4 Synthesis of the alkaloid pseudopelletierene.

Reference books:

1. Organic Synthesis, V. K. Ahluwalia and R. Aggarwal, Narosa Publishing House, N. Delhi, 2001.
2. Microwaves in Organic Synthesis, Andre Loupy (Ed.), Wiley – VCH Verlag, Weinheim, 2002.
3. Experimental plastic technology- J A Brydson and K J Saunders, Methun E L, 1970
4. Polymer Synthesis: Theory and Practice- Fundamentals, Methods, Experiments, - D. Braun • H. Cherdron • M. Rehahn • H. Ritter • B. VoitFourth Edition, Springer
5. Organic Photochemistry, J Kopckey, VCH Publishers, 1992.
6. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
7. D.W. Mayo, R.M. Pike and P.K. Trumper, Microscale Organic Laboratory, John Wiley and Sons, Inc., ISBN 0-471-57505-4, 3rd edition, 1994
8. D.L. Pavia, G.M. Lampman and G.S. Kriz, Introduction to Organic Laboratory Techniques, Saunders College Publishing, ISBN 0-03-006232-2, 2nd edn 1995
9. O.R. Rodig, C.E. Bell, Jr., A.K. Clark, Organic Chemistry Laboratory, Saunders College Publishing, ISBN 0-03-012644-4, 1990
10. K.L. Williamson, D.C. Heath and Co. Macroscale and Microscale Organic Experiments, ISBN 0-669-24369-9, 2nd edition, 1994

CHOO-510 Laboratory course in Medicinal Chemistry (2 credits)

Minimum 10 experiments of 6 hrs duration each. It is mandatory that the concerned teacher sensitizes the students on the theoretical aspects/considerations of each experiment before asking the students to carry out the same. The students are required to undertake pre-lab. and post – lab. assignment as instructed by the concerned teacher and the same may be evaluated by according suitable weightage as an ISA component while prescribing the mode of assessment.

1. Quantitative estimations (expt. No. 1 is compulsory. Out of remaining ones, any four estimations are to be carried out).

1. Streptomycin using U V – visible spectrometer.
2. Ascorbic acid by ceric ammonium sulfate method.
3. Paracetamol by hydrolysis.
4. Phenacetin by diazotization procedure.
5. Free fatty acids in oil / fat.
6. Protein by UV absorption method.
7. Amino acids using ninhydrin method.
8. Thiamine assay of Vitamin B Complex tablets.
9. Assay of Belladona for Hyoscyamine.

2. Preparation of simple drugs (any five).

1. Phenacetin / Acetaminophen from *p*-aminophenol.
2. Aspirin from salicylic acid.
3. Barbiturate from diethyl *n*-butyl malonate
4. Benzocaine from *p*-aminobenzoic acid.
5. 4- methyl – 7 – hydroxy coumarin.
6. Sulphanilamide from acetanilide.

3. Isolation and transformation (any three)

1. Isolation of cholesterol from gallstones.
2. To demonstrate the enzyme activity in salivary digestion.
3. Transformation of Benzaldehyde to benzoin using thiamine (B_1) as a coenzyme.
4. Isolation of caffeine, the purine class of alkaloid from tea.

4. Separation / identification of individual components in a commercial drug preparation using TLC (any one).

1. Sulfonamides in a sulfa drug tablet.
2. Analgesics in an analgesic tablet.

5. Some color tests / reactions of following group of compounds (any five types)

carbohydrate, cholesterol, fat-soluble vitamins, alkaloids, glycosides, tannins and antibiotics.

Reference Books :

1. Medicinal Chemistry Laboratory Manual: Investigations in Biological and Pharmaceutical Chemistry, Charles Dickson, CRC Press, New York, 1999.
2. Practical Organic Chemistry, F. G. Mann and B. C. Saunders, Orient Longman, 4th edition.
3. Elementary Practical Organic Chemistry, Part III – Quantitative Organic Analysis, A. I. Vogel, CBS Publishers, New Delhi.
4. Organic Analytical Chemistry, Jag Mohan, Narosa Publishing House, N. Delhi, 2003.
5. Macroscale and Microscale Organic Preparation, K.L.Williamson, D.C.Heath and Co., 1989.

CHOO-511 Green Chemistry Techniques in Organic Synthesis (3 credits)

1. Designing a green synthesis (4)

1.1 . Introduction

1.2 . Choice of starting materials, reagents, catalysts and solvents.

1.3 . Basic principles of green techniques.

1.4 . Green chemistry in day – to – day life.

2. Organic Synthesis and Environmental Pollution (5)

2.1 . Introduction

2.2 . Green reagents : Dimethyl carbonate and Polymer supported reagents.

2.3 . Green catalysts : Acid and basic catalysts, Oxidation catalysts and Polymer supported catalysts.

2.4 . Aqueous phase reactions and photochemical reactions.

3. Phase Transfer Catalysis in green synthesis. (3)

3.1 . Introduction, definition and mechanism of PTC reactions.

3.2. Types of Phase Transfer catalysts, PT reactions and advantages.

3.3. Crown ethers : Nomenclature and special features.

3.4. Application of Phase transfer catalysis in green synthesis.

4. Microwave induced green synthesis. (3)

4.1 . Introduction, Microwave technology and equipment microwave ovens and reactors, advantages limitations and precautions to be taken.

4.2 . Microwave assisted reactions in water and organic solvents.

4.3 . Solvent free (solid state) reactions.

5. Ultrasound assisted synthesis. (3)

5.1 . Introduction, Instrumentation, physical aspects and types of sonochemical reactions.

5.2 . Synthetic applications of ultrasound.

6. Biocatalysts in organic synthesis. (3)

6.1 . Introduction, Biochemical oxidations and reductions.

6.2 . Enzymes catalysed hydrolytic processes.

7. Organic synthesis in solid state. (4)

7.1 . Introduction, Solvent free synthesis.

7.2 . Solid supported organic synthesis - General techniques, supports and linkers for solid phase synthesis, advantages of polymer supported reagents.

7.3 . Synthetic applications.

8. Ionic liquids as green solvents. (3)

8.1 . Introduction, Reactions in acidic Ionic liquids.

8.2 . Reactions in neutral Ionic liquids : Hydrogenation, Diels – Alder, Heck

reaction, O - and N - alkylation and methylene insertion reaction.

9. Chemical synthesis using supercritical fluids. (4)

9.1 . Introduction, Supercritical Fluids (SCF) as media for chemical reactions.

9.2 . Practical aspects of reactions, Phase behaviour and solubility, Industrial uses of SCF's as reaction media.

9.3 . Extraction, separation, precipitation, crystallisation and microemulsion techniques.

9.4 . Stoichiometric organic reactions in SCF.

10. Synthesis involving basic principles of green chemistry : Some examples. (4)

Reference books.

1 Introduction to Green Chemistry, Albert S. Matlack, Marcel Dekker, Inc., New York, 2001.

2 Green Chemistry: Frontiers in benign chemical synthesis and processes, Paul T. Anastas and Tracy C. Williamson (Eds.), Oxford University Press, Oxford, 1998.

3 Green Chemistry: Environmentally Benign Reactions, V. K. Ahluwalia, Ane Books India, New Delhi, 2006.

4 New Trends in Green Chemistry, V. K. Ahluwalia and M. Kidwai, Anamaya Publishers, N. Delhi, 2004.

5 Chemical Synthesis using Supercritical fluids, P. G. Jessop and W. Leitner (Eds.), Wiley – VCH, Verlag, Weinheim, 1999.

6 Organic Synthesis, V. K. Ahluwalia and R. Aggarwal, Narosa Publishing House, N. Delhi, 2001.

7 Solvent Free Organic Synthesis, Koichi Tanaka, Wiley – VCH GmbH and Co. KgaA, Weinheim, 2003.

8 Green Chemistry, Theory and Practice, P. T. Anastas and J. C. Warner, Oxford University Press, N. York, 1998.

9 Organic Reactions in aqueous Media, C - Jun Li and T – Hang Chan, John Wiley and Sons INC., N. York, 2001.

10 Organic Synthesis on Solid Phase, F. Z. Dorwald, Wiley – VCH Verlag, Weinheim, 2002.

11 Ionic Liquids in Synthesis, Peter Wasserscheid and Tom Welton (Eds.), Wiley – VCH Verlag, Weinheim, 2003.

12 Microwaves in Organic Synthesis, Andre Loupy (Ed.), Wiley – VCH Verlag, Weinheim, 2002.

13 High Pressure Chemistry, R. Van Eldik and F. G. Klarner (Eds.), Wiley – VCH Verlag, Weinheim, 2002.

14 Green Chemistry, Samuel Delvin, IVY Publishing House, Delhi, 2006.

CHOO-512 Laboratory course on Green Chemistry Techniques in Organic Synthesis (2 credits.)

Minimum 10 experiments of 6 hrs duration each. It is mandatory that the concerned teacher sensitizes the students on the theoretical aspects/considerations of each experiment before asking the students to carry out the same. The students are required to undertake pre-lab. and post – lab. assignment as instructed by the concerned teacher and the same may be evaluated by according suitable weightage as an ISA component while prescribing the mode of assessment.

1. Enzymatic transformations (any one).

a) *S* (+) Ethyl – 3 – hydroxy butanoate from ethylacetoacetate using bakers yeast.
b) Deoximation of p-methoxy benzaldehyde oxime by ultrasonically stimulated baker's yeast.
c) Reduction of acetophenone to 1-phenyl (1*S*)-ethan-1-ol using *Daucus carota* (carrot) root.
d) Benzaldehyde to benzoin by using biological coenzyme thiamine hydrochloride catalyst.
e) Chiral reduction of EAA to (*S*)-(+)-ethyl-3-hydroxybutanoate by using baker's yeast.

2. Phase transfer catalysis (PTC) (any three).

a) Darzens condensation of cyclohexanone with chloroacetonitrile to provide 1-oxaspiro-[2,5]-octane-2-carbonitrile.
b) *Syn* – hydroxylation of cyclooctene or cyclohexene with $KMnO_4$ solution.
c) Oxidation of benzyl alcohol with hypochlorite solution.
d) 3,4-diphenyl-7-hydroxycoumarin by the reaction of 2-hydroxy-4-methoxy benzophenone with phenylacetyl chloride.
e) Flavone from o-hydroxyacetophenone and benzoylchloride.
f) 2,2-dichlorobicyclo[4.1.0]heptane from cyclohexene and chloroform in presence of NaOH.
g) Toluene to benzoic acid by alkaline KMnO4.
h) Salicylaldehyde from phenol and chloroform.

3. Solvent free synthesis (any one).

a) Claisen rearrangement of allylphenyl ether to 2-allyl phenol.
b) Synthesis of dicoumarol.
c) *N* – alkylation of saccharin by microwave irradiation.

4. Microwave assisted synthesis (any one).

a) Synthesis of tetrapyrrolic macrocycle under dry media conditions with microwave activation from benzaldehyde and pyrrole.
b) Synthesis of 1,4 – dihydropyridine in presence of silicagel under microwave irradiation from substituted aldehydes and ethylacetoacetate.
c) 3-Methyl-1-phenyl-5-pyrazolone from EAA and phenylhydrazine.
d) DA reaction of anthracene with maleic anhydride.

5. Ionic liquids in synthesis (compulsory).

a) FC reaction of naphthalene with acetyl chloride in presence of [emin]Cl-$AlCl_3$ at room temperature.

6. Ultrasound in synthesis (any two).

a) Coupling reaction between a □□, □ – unsaturated carbonyl compound and acetone.

b) Aldol dimerisation of □□– tetralone catalysed by basic alumina.

c) 2-chloro-N-aryl anthranilic acid from 2-chlorobenzoic acid and 2-chloroaniline.

d) Butyraldehyde from 1-chlorobutane by the reaction of Li and dimethyl formamide.

7. Aqueous phase reaction (any two).

a) Alkylation of active methylene group by the use of dimethyl carbonate in presence of potassium carbonate.

b) Michael addition of cyclohexenone to ascorbic acid.

c) Michael addition reaction of chalcone and ethylacetoacetate.

d) Chalcone from benzaldehyde and acetophenone.

e) *trans*-Stilbene from benzaldehyde and benzyltriphenyl phosphonium-chloride.

f) Claisen – Schmidt reaction of acetophenone with benzaldehyde using phase transfer catalyst.

g) Sodium borohydride reduction of carbonyl compounds.

8. Photochemical reactions (any two).

a) Dimerization of cinnamic acid to truxillic acid.

b) Cyclisation of coumarin derivative in solid state / water.

c) Benzopinacol by reduction of benzophenone in isopropyl alcohol.

d) Isomerisation of trans-azobenzene to cis-azobenzene.

9. Solid state reactions (any two).

a) $NaBH_4$ reduction of benzophenone to diphenyl carbinol.

b) Phenylbenzoate by BV oxidation of benzophenone.

c) 3-pyridyl-4(3H)quinazolone from anthranilic acid, formic acid and 2- aminopyridine using MW irradiation.

d) Citronellal from citronellol using PCC on alumina.

Reference books.

1. Green Chemistry: Environmentally Benign Reactions, V. K. Ahluwalia, Ane Books India, New Delhi, 2006.
2. New Trends in Green Chemistry, V. K. Ahluwalia and M. Kidwai, Anamaya Publishers, N. Delhi, 2004.
3. Organic Synthesis, V. K. Ahluwalia and R. Aggarwal, Narosa Publishing House, N. Delhi, 2001.
4. Solvent Free Organic Synthesis, Koichi Tanaka, Wiley – VCH GmbH and Co. KgaA, Weinheim, 2003.

5. Green Chemistry, Theory and Practice, P. T. Anastas and J. C. Warner, Oxford University Press, N. York, 1998.
6. Organic Reactions in aqueous Media, C - Jun Li and T – Hang Chan, John Wiley and Sons INC., N. York, 2001.
7. Organic Synthesis on Solid Phase, F. Z. Dorwald, Wiley – VCH Verlag, Weinheim, 2002.
8. Ionic Liquids in Synthesis, Peter Wasserscheid and Tom Welton (Eds.), Wiley – VCH Verlag, Weinheim, 2003.
9. Microwaves in Organic Synthesis, Andre Loupy (Ed.), Wiley – VCH Verlag, Weinheim, 2002.
10. Green Chemistry, Samuel Delvin, IVY Publishing House, Delhi, 2006.
11. Introduction to Green Chemistry, Albert S. Matlack, Marcel Dekker, Inc., New York, 2001.
12. Green Chemistry: Frontiers in benign chemical synthesis and processes, Paul T. Anastas and Tracy C. Williamson (Eds.), Oxford University Press, Oxford, 1998.

M Sc-Part II Physical chemistry
Semester III and IV Courses

Compulsory courses			**Optional courses**		
Code	**Title**	**Credits**	**Code**	**Title**	Credits
CHPC–501	Quantum Chemistry and Spectroscopy	**4**	CHPO-501	Colloids and Surface Science	4
CHPC–502	Advanced Thermodynamics and Kinetics	**4**	CHPO-502	Solid State Chemistry: Concepts and Applications	4
CHPC–503	Electrochemistry	**4**	CHPO-503	Advances in Catalysis	4
CHPC–504	Experiments in Physical Chemistry	**4**	CHPO-504	Nanoscience : Concepts and Applications	4
			CHPO-505	Lab Course in Applied Chemistry	4
			CHPO-506	Lab Course in Physical Chemistry – I	8
			CHPO-507	Computational Chemistry	2
			CHPO-508	Radiation Chemistry	2
			CHPO-509	Applied Electrochemistry	2
			CHPO-510	Biophysical Chemistry	2
			CHPO-511	Dissertation	8
			General Optional Courses		
			CHGO-501	Biological Chemistry	4
			CHGO-502	Green Chemical Processes	2
			CHGO-503	Chromatographic Methods	2
			CHGO-504	Conventional and Non-Conventional Energy	2

CHPC-501: Quantum Chemistry and Spectroscopy (4 Credits)

1. Quantum Chemistry (45)

1.1 The origin of quantum mechanics: Planck's quantum theory, wave particle duality, uncertainty principle concept of wave function, the Born interpretation of wave function. Normalization and orthogonalizations, quantisation, Eigen values and Eigen functions.

1.2 Postulates of quantum mechanics; Schrödinger equation for free particle, particle in a box, degeneracy. Quantum mechanical operators and their properties, commutation relations, Hamiltonian and Laplacian operators, Harmonic oscillators, Angular momentum, Ladder Operators.

1.3 Approximate methods, Schrödinger equation, its importance and limitations, Born-Oppenheimer approximation, Anti-symmetric wave functions and Slater determinants (many electron system e.g. He atom), Exclusion and Aufbau principle, Variation method, Linear Variation Principle, Perturbation theory (first order non-degenerate) and their applications to simple systems; term symbols and spectroscopic states.

1.4 VB and MO theory, Huckel MO theory, Bond-order, Charge density matrix, Unification of HMO and VB theory, their applications in spectroscopy and chemical reactivity, electron density forces and their role in chemical bonding. Hybridization and valence MOs of H_2O, NH_3 and CH_4. Application of Huckel Theory to ethylene, butadiene and benzene molecules. Introduction to Extended Huckel Theory, Idea of self-consistent fields.

2. Elements of Group Theory (20)

2.1 Symmetry elements and symmetry operations, Concept of group and group multiplication tables, Classes and subgroups in a group, Different types of groups (cyclic, abelian and non-abelian), Point groups, Reducible and Irreducible representations, Properties of Irreducible representations, Great Orthogonality Theorem, Character tables, Space groups, Bravais lattices.

2.2 Group Theory and Quantum Chemistry: Vanishing of integrals, Selection rules for Vibrational, Electronic, vibration and Raman spectra, Symmetry adapted linear combinations (SALCs), MO treatment of large molecules with symmetry.

3. Microwave, IR and Raman Spectroscopy (10)

3.1 Theoretical treatment of Rotational and Vibrational spectroscopy.

3.2 FTIR spectroscopy Theory, instrumentation and applications.

3.3 Quantum theory of Raman effect, Raman shift, Instrumentation, Resonance Raman spectroscopy, Complimentary nature of IR and Raman spectroscopy in structure determination, Applications.

4. NMR Spectroscopy (13)

4.1 Basic principles of NMR.

4.2 Theory of pulse NMR and Fourier analysis, FT-NMR.

4.3 Solid state NMR, magic angle spinning (MAS), dipolar decoupling and cross polarization, applications of solid state NMR.

4.4 Double resonance, NOE, Spin tickling, Solvent and shift reagents, Structure determination by NMR.

5. ESR Spectroscopy (12)

5.1 Theory and experimental techniques, Identification of odd-electron species (methyl and ethyl free radicals) and radicals containing hetero atoms.

5.2 Spin trapping and isotopic substitution, Spin densities and McConell relationship, Double resonance techniques.

** Number shown in brackets indicate percentage weightage*

TEXT BOOKS:

1. Atkins' Physical Chemistry 8th Ed., P.W. Atkins and J. De. Paulo, Oxford Univ. Press (2007)
2. Quantum Chemistry 4th Ed., Ira. N. Levine, Prentice-Hall, New Delhi (1995).
3. Introductory Quantum Chemistry A.K. Chandra, Tata McGraw Hill, New Delhi, (1992).
4. Coulson's Valence, R. McWeeny, ELBS, Britain (1979).
5. Chemical Applications of Group Theory 3rd Ed., F.A. Cotton, John Wiley and sons-Asia, New Delhi (1999).
6. Group Theory and its applications to chemistry, K. V. Raman, Tata McGraw-Hill, New Delhi
7. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. McCash, Tata McGraw-Hill, New Delhi, 1994.
8. NMR in Chemistry a multinuclear introduction, W. Kemp, Macmillan (1986).
9. Physical Methods in Chemistry, R.S. Drago, W.B. Saunders Company (1977).
10. Physical Chemistry, Donald A. McQuarrie and John D. Simon, Viva Books Pvt. Ltd., New Delhi

CHPC-502: Advanced Thermodynamics and Reaction Kinetics (4 Credits)

1. Equilibrium Thermodynamics: (**16)**

1.1 Thermodynamic state functions. Exact and inexact differentials, partial derivatives, Maxwell relations.

1.2 Thermodynamic equations of state. Temperature and pressure dependence of Gibbs function. Gibbs-Helmholtz equation. Partial molar quantities. Free energy change accompanying a chemical reaction, chemical potential, Gibbs-Duhem equation. Duhem-Margules equation.

1.3 Entropy of mixing for gases and liquids. Gibbs paradox, Thermodynamic derivation of phase rule

2. Statistical Thermodynamics: (34)

2.1 The language of statistical thermodynamics: Probability, ensemble, macrostate, microstate, degeneracy, permutations and combinations. Configuration and weights, the dominant configuration. The Boltzmann distribution. The molecular partition function: its interpretation and its relation to uniform energy levels.

2.2 Translational, Rotational, Vibrational and Electronic Partition functions for diatomic molecules. Relation between thermodynamic functions and partition functions and their statistical interpretations. Equilibrium constants from partition function.

2.3 Law of Equipartition energy. Theories of specific heat of solids. Comparison between Einstein and Debye theories.

3.4 Concept of symmetric and antisymmetric wave functions. Ortho and para hydrogens. Quantum Statistics: Fermi-Dirac (FD)and Bose-Einstein (BE) statistics. Comparison between MB, FD and BE Statistics.

3. Non-equilibrium Thermodynamics: (**20)**

3.1 Concept of internal entropy and spontaneity of a process in relation to free energy. Chemical affinity and extent of a reaction. Mass and energy balance equations. Entropy production in heat flow, chemical reactions and open system.

3.2 Postulates and methodologies, linear laws, Gibbs equations, Onsager's reciprocal theory. Validity of Onsager's equation and its verification. Application to thermo-electric and electro-kinetic phenomena.

4. Reaction Kinetics: (30)

4.1 Collision theory of reaction rates and treatment of unimolecular reactions. Theory of absolute reaction rates and its applications to reactions in solution. Thermodynamic study from reaction kinetics, comparison of results with Eyring and Arrhenius Equations. Solvent and salt effects; influence of ionic strength and solvent on the rates of reaction, primary and secondary salt effects.

4.2 Mechanism of photochemical, chain, coupled and Reversible reactions. Oscillatory reactions. Chemical Hysteresis in Belousov-Zhabotinskii reaction.

4.4 Fast reactions and study by stopped flow technique, relaxation method, pulse radiolysis, flash photolysis and magnetic resonance methods.

4.5 Homogeneous catalysis and Michaelis-Menten kinetics. Kinetic rate law for autocatalytic reactions. Kinetics of heterogeneous reactions, heterogeneous catalysis, inhibition, product induced and non–reactive inhibition.

4.6 Potential energy surfaces and introduction to molecular reaction dynamics, theoretical calculation of energy of activation, chemical lasers.

TEXT BOOKS:

1. Atkins' Physical Chemistry 8th Ed., P.W. Atkins and J. De. Paulo, Oxford Univ. Press (2007)
2. Thermodynamics For students of Chemistry, Classical, Statistical and Irreversible, J. Rajaram and J.C. Kuriacose, S.N. and Co., Jalandhar, 1996.
3. Fundamentals of Chemical Thermodynamics, by E. N. Yeremin.
4. Statistical Thermodynamics, M.C. Gupta Wiley Eastern, New Delhi, (1990).
5. Statistical Mechanics, Kerson Huang, IInd Ed., Wiley India Edition
6. Physical Chemistry, Statistical Mechanics, Horia Metiu, Taylor and Francis, New York (2006).
7. Chemical Kinetics, K.J. Laidler, Tata McGraw, New Delhi (1985).
8. Physical Chemistry, Donald A. McQuarrie and John D. Simon, Viva Books Pvt. Ltd., New Delhi

REFERENCE BOOKS:

1. Advanced Thermodynamics, P. C. Rakshit, Science Book Agency.
2. Physical Chemistry, by G.W Castellan, Narosa Publishing house, New Delhi (1994).
3. Text Book of Physical Chemistry/Chemical Thermodynamics, S. Glasstone, Van Nonstrand.
4. Elements of Statistical Thermodynamics, L.K. Nash, Addison-Wesley, Menlo Park, (1972).

CHPC – 503: ELECTROCHEMISTRY (4 credits)

1. Electrolyte Solutions (24)

1.1 Ion-solvent interactions. Born Theory: Its validity and limitations.
1.2 Difference between solvation number and coordination number.
1.3 Ion-ion interactions and Debye-Huckel theory of ionic atimosphere.
1.4 Concept of ionic strength, activity coefficient and its determination.
1.5 Debye-Huckel limiting law and its modifications.
1.6 Ion-association, Transport of ions in solutions.
1.7 Laws of diffusion, Diffusion coefficient.
1.8 Einstein-Smoluchowski equation.
1.9 Ionic mobility and transport number.
1.10 Debye-Huckel-Onsager equation of conductance, its validity and limitations.
1.11 Concepts of proton transport in solutions.

2. Electrified Interfaces (16)

2.1 Formation of an electrified interface and its structure.
2.2 Polarizable and non-polarizable interfaces.
2.3 Concepts of outer potential, surface potential, inner potential and relationship between them, chemical and electrochemical potentials.
2.4 Concept of surface excess, Electro-capillary curves.
2.5 Condition for thermodynamic equilibrium at electrified interface.
2.6 Surface phase and Gibbs adsorption equation. Surface tension and adsorption on solid. Generalized Gibbs equation, Lippmann equation and capacity of the double layer.
2.7 Determination of surface excess, Models for the electrified interface.
2.9 Contact adsorption and its evaluation, influence of contact adsorption on capacity of interface. Adsorption isotherms.

3. Electrode Kinetics and Corrosion (20)

3.1 Disturbance of electrode equilibrium, cause of electron transfer, fast and slow systems and their current-potential relationship.
3.2 Butler-Volmer equation and its low and high field approximations.
3.3 Nernst equation as a special case of B-V equation. Applications of Nernst equation.
3.4 Tafel plots for anodic and cathodic processes.
3.5 Multi-step reactions and determination of stepwise mechanism of electrodic reactions.
3.6 Study of pH-potential diagrams.
3.7 Principles of corrosion, corrosion prevention, corrosion testing.
3.8 Pourbaix diagram for corrosion.

4. **Membranes, Colloids and Mircoemulsions. (20)**

4.1 Charge and Stability of Sols. DLVO theory
4.2 Electrokinetic phenomena: Electroosmosis, streaming potential and current, electrophoresis. Zeta potential and its determination.
4.3 Donnan membrane equilibria

4.4 Micelles and reverse micelles: solubilisation, and bilayers.
4.5 Microemulsions: (formation, phase diagrams, composition and structure).
4.6 Diffusion and Osmosis
4.7 Structure of Biomembranes: lipid bilayers and membrane proteins. Structure of biopolymers.
4.8 Transport of substances across cell membranes. Role of voltage and ligand gated channels. 4.8 Role of Na^+/K^+ ATP-ase

5. **Electrochemical Energies** **(20)**

5.1 Thermodynamics of electrochemical energy conversion.
5.2 Batteries: basic principles; types of batteries: basic battery elements, battery characteristics: energy density, rating and shelf life etc. Zinc-manganese dioxide: Leclanche, alkaline and rechargeable batteries. Lead-acid battery in relation to other storage batteries; determination of state of charge in batteries. Principle of solid state batteries. Lithium ion batteries
5.3 Principles of solid electrolytes and evaluation of their impedance through complex impedance diagrams.
5.4 Fuel cells: Principle of a hydrogen-oxygen fuel cell. Classification of fuel cell systems. Efficiency vis-à-vis thermodynamic efficiency, reliability and economic benefits; Fuel cells and their applications. Direct methanol-polymer electrolyte fuel cell and electrocatalysts - a case study.
5.5 Hydrogen as a fuel: methods of production, storage principles, transportation and safety aspects.
5.6 Photo-electrochemical energy conversion at semiconductor/electrolyte interface, photo-electrolysis cell.
5.7 Supercapacitors: Introduction: Origin of supercapacitance. Aqueous systems – ruthenium oxide/carbon with sulphuric acid and or solid polymer electrolytes.

Text Books:

1. Modern Electrochemistry: by J.O.M. Bockris and A.K.N. Reddy, Vol. 1, 2 and 3, Plenum,
2 Principles and Applications of Electrochemistry, by D.R. Crow, Blaki Academic, London

Reference Books:

1. Electrochemical Science; J.OM. Bockris and D.M. Drazic
2. Electrochemistry: Principles, methods and applications, by C.M.A. Brett and A.M.O. Brett, Oxford Univ. Press, Oxford
3. Colloid and Interface Chemistry, by R.D. Vold and M.J. Vold, Addison-Wesley, Reading (1983).
4. Solid State Chemistry and its Applications by A.R. West, John Wiley and Sons, Singapore.
5. Modern Batteries, A. Vincent, B. Sacrosati, 1997, John Wiley, New York.
6. Fuel cells: their Electrochemistry, J.O. M. Bockris and S. Srinivasan McGraw-Hill Book Co.,
7. Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications" by B.E. Conway, Plenum Publication Corp. (paperback).

CHPC – 504: Experiments in Physical Chemistry (4 credit)

Group - A. Instrumental

I1- To determine the energy of activation of reaction of
$Zn + PbSO_4 \text{ ----> } ZnSO_4 + Pb$ potentiometrically.

I2- To determine the instability constant of the reaction
$[Ag(NH_3)_2] \text{----> } Ag + 2NH_3$ potentiometrically

I3- To study the electrokinetics of rapid reaction between SO_4^{2-} and I^- in an aqueous solution.

I4- To verify Nernst equation and determine the standard oxidation potential of copper and zinc ion electrodes.

I5- To study effect of ionic strength on activity coefficient of Ag^+ ions.

I6- To study spectrophotometric titration of ferrous ammonium sulphate with potassium permanganate (or dichromate vs permanganate)

I7- To investigate the reaction kinetics between potassium persulphate and potassium Iodide colorimetrically.

I8-To determine the equivalent conductance of a strong electrolyte at several concentrations and verify Onsager's equation.

I9- To estimate the concentration of sulphuric acid, acetic acid and copper sulphate in a given solution conductometrically.

I10- To determine the concentration of Fe(II) ions by titrating with potassium dichromate conductometrically.

I11- To verify Tafel Relationship.

I12- To determine the throwing power of the given plating bath by electrodeposition.

I13- To study the kinetics of hydrolysis of tertiary butyl chloride by conductometry

I14- To determine the back EMF, ir drop and decomposition potential during electrolysis

I15- To determine the half wave potential of Cu^{2+}/Cd^{2+} /Zn^{2+} by using polarography

Group - B. Non-Instrumental

N1- To determine the partial molal volume of ethanol-water mixture at a given temperature

N2-To study the phase rule for two component system

N3-To determine the partial molal volume of sodium chloride-water, ethanol-water and methanol-water system (apparent molal volume method)

N4- To determine the effect of salt on surface tension of water using by capillary rise method

N5- To study effect of surfactants on surface tension of water using stalagmometer

N6- To study the variation of viscosity with composition of mixtures and to verify the formation of compounds by Oswald's viscometer

N7- To study the effect of pH on the kinetics of iodination of aniline

N8- To study the kinetics of reaction between H_2O_2 and KI (clock reaction)

N9- To study the kinetics of rapid reaction between bromine and iodine in aqueous media

N10- To investigate the autocatalytic reaction between potassium permanganate and oxalic acid.

N11- To study the electroless deposition of Ni on non-conductor substrate and to determine the rate of deposition

N12- To study the acid and alkaline corrosion susceptibility of metal and to determine the rate of corrosion

N13- To study the catalytic activity of three different metal oxides in heterogeneous systems with H_2O_2 decomposition reaction

N14- To determine the molecular weight of a polymer by intrinsic viscosity method.

Group - C. Computational Chemistry

C1- To generate a mark sheet to learn various features of spreadsheets (revision)

C2- To generate a plot for a given function (like solutions of 1D box, harmonic oscillator, H-like atom wave functions, Gaussians distributions etc) (revisions)

C3- To write a computer program to obtain equivalence point in pH metry and potentiometric experiments (derivative method)

C4- To write a computer program to find percent composition for various atoms of a given molecular formula

C5- To write a computer program to obtain slope and intercept for linear data using least square fit method

C6- To write a computer program to obtain centre of mass of a given molecule and moment of inertia, hence obtain classification of the given molecule

C7- To write a computer program to find out various parameters for data analysis viz. minimum, maximum, average, standard deviation, variance, covariance, correlation coefficient, frequency distribution etc.

C8-To write a computer program to obtain thermodynamic probability.

C9-To write a computer program to obtain degeneracy of a given energy level for a particle in a cube.

(Note: minimum 6 experiments to be performed from each group and one independent experimental/computational assignment on a particular theme of 10 CH each OR 9 - 12 experiments each from Group A and group B and 6 experiments from group C)

CHPO – 501: Colloids and Surface Science (4 credit)

1. Liquid Surfaces and Interfaces (18)

1.1 General Introduction. Microscopic picture of liquid surface.

1.2 Surface tension and its measurement. Curved liquid surfaces.

1.3 The Kelvin equation and capillary condensation.

1.4 Nucleation Theory.

1.5 The surface excess. Gibbs energy and surface tension. The surface tension of pure liquids. Gibbs adsorption isotherm.

1.6 Gouy – Chapman Theory and Grahame equation. The Stern layer and Gibbs free energy of the double layer.

2. Electrokinetic Phenomena and Surface Forces (20)

2.1 Electrocapillarity – theory and measurement.

2.2 Charged surfaces such as mercury, silver iodide and oxides. Measurement of surface charge densities.

2.3 Electrokinetic phenomena: concept of zeta potential. Electroosmosis and streaming potential. Electrophoresis and sedimentation potential.

2.4 Surface forces – Van der Waals forces between molecules. Surface energy and Hamaker constant. Measurement of surface forces. The DLVO theory and beyond.

Contact angle and its measurements. The line tension. Wetting and wetting transitions. Important wetting geometries. Wetting and dewetting.

3. Solid Surfaces (20)

3.1 Description of crystalline surfaces

3.2 Preparation of clean surfaces.

3.2 Surface stress and surface tension. Determination of surface energy. Surface steps and defects

3.3 Solid – solid interfaces

3.4 Microscopy of Solid surfaces: Optical microscopy, Electron Microscopies, Scanning Probe Microscopy (STM, AFM).

3.5 Diffraction Methods.

3.6 Spectroscopic methods (XPS, UPS, AES, EDX, SIMS)

4. Adsorption (16)

4.1 Types of adsorption and adsorption times. Classification of adsorption isotherms.

4.2 Thermodynamics of adsorption.

4.3 Adsorption Models. The potential theory of Polanyi.

4.4 Experimental aspects of adsorption from gas phase.

4.5 Adsorption on porous solids.

4.6 Adsorption from solution.

5. Surface Modification (6)

5.1 Chemical vapour deposition

5.2 Soft matter deposition: self-assembled monolayers, physisorption of polymers, polymerization on surfaces

5.3 Etching techniques 5.4 Lithography, surface elasticity and viscosity.

6. Surfactants, Micelles, Emulsions and Thin films (20)

6.1 Classification of surfactants.

6.2 Spherical micelles: cmc and influence of temperature. Thermodynamics of micellization. Structure of surfactant aggregates

6.3 Macroemulsions: properties, formation and stabilization. Evolution and aging. Coalescence and demulsification.

6.4 Microemulsions: size of droplets. Elastic properties of surfactant films. Factors influencing the structure of microemulsions.

6.5 Thin films on surfaces of liquids:Introduction and phases. Optical and X-Ray methods to study monolayers.

6.6 The surface potential

6.7 Langmuir Blodgett Transfer

Text Book

1. H J Butt, K. Graf and M. Kappl, Physics and Chemistry of Interfaces, Wiley-VCH

Reference Books

1. A.W. Adamson and A.P.Gast, Physical Chemistry of Surfaces

2. D. Myers, Surfaces, Interfaces and Colloids 3. R.D. Vold and M.J. Vold, Colloid and Interface Chemistry, by Addison-Wesley, Reading

CHPO – 502: Solid State Chemistry: Concepts and Applications (4 credits)

1. Solid State Reactions: (10)

1.1 General Principles and experimental procedure.
1.2 Methods of preparing fine particle simple and mixed metal oxides such as precursor, sol-gel etc.
1.3 Ion exchange and intercalation reactions.
1.4 Preparation of thin films. Hydrothermal synthesis.

2. X – Ray Diffraction: (16)

2.1 Unit Cells, symmetry, point groups and space groups.
2.2 Miller Indices, lattice planes, d-spacings and multiplicities.
2.3 The X-ray diffraction experiment: powder and single crystal methods.
2.4 Intensities: scattering of X-Rays and factors that affect intensities.
2.5 R-factors and structure determination. Electron density maps.
2.6 Particle size measurements.
2.7 Refinement of unit cell parameters and indexing of powder patterns.

3. Point Groups and Space Groups: (10)

3.1 Representation of point groups. Point symmetry of molecules.
3.2 Space groups: triclinic, monoclinic, orthorhombic, tetragonal.
3.3 Space groups and Crystal structures: perovskite and rutile type

4. Crystal Chemistry: (10)

4.1 Close packed structures-ccp and hcp.
4.2 Ionic structures and tetragonal packing.
4.3 Structures built of space filling polyhedra.
4.4 Some important structure types – rock salt, zinc blende, wurtzite, nickel arsenide and rutile.

5. Factors that Influence Crystal Structures: (14)

5.1 general formulae, valencies and coordination numbers. Effect of bonding and atomic sizes.
5.2 ions and ionic radii. Radius ratio rules
5.3 lattice energy of ionic crystals.
5.4 The Born-Haber cycle and thermochemical calculations.
5.5 non bonding electron effects.

6. Crystal Defects and non stoichiometry: (8)

6.1Types of defects. Point defects and thermodynamics.
6.2 Colour Centres.
6.3 Vacancies and interstitials in non stoichiometric crystals.
6.4 dislocations, mechanical properties and reactivity of solids.

7. Phase Diagrams and Phase Transitions: (14)

7.1 Basic Concepts and definitions.
7.2 Three component condensed systems. Thermodynamics and kinetics of phase transitions. Martensitic transformations. Order-disorder transitions.

8. Ionic Conductivity and Solid Electrolytes: (**8)**

8.1 General Introduction 8.2 conduction in NaCl and AgCl
8.3 Fast ion conductors and conductivity measurements by DC and AC methods.

9. Electronic Properties and Band Theory: (**10)**

9.1 Electronic structure and band theory of solids.
9.2 Band structure of metals and semiconductors. Controlled valency semiconductors.
9.3 Formation of acceptor and donor levels and diagram of pn junction.
9.4 Band structure of inorganic solids with suitable examples. Magnetic properties of transition metal oxides and spinels. Smart materials and applications

Text Book

1. A. R. West, Solid State Chemistry and Its Applications (Wiley – India)

Reference Books

1. H. V. Keer, Principles of the Solid State and Applications

**(the course content and credit weightage for CHPO-502 and CHIC-502 are to be treated equivalent)*

CHPO - 503: Advances in Catalysis (4 credits)

1. Basic Concepts: (30)

General Introduction: Catalysis and activation energy. Homogeneous and heterogeneous reactions with suitable illustrations. Catalytic activity. selectivity and stability. Types of catalytic reactors. Steps in a heterogeneous catalytic reaction. Factors affecting rate of reaction such as temperature, flow rates, molar composition etc. TOF in catalysis.

Adsorption and Surface Area: Cause of adsorption. No of molecules striking the surface and sticking probability. Types of adsorption and potential energy profiles for adsorption of H_2. Adsorption isotherms for gases and solutes. Basic types of BET isotherms. Gibbs adsorption equation and changes in surface tension. Free energy, enthalpy and entropy of adsorption. Chemisorption of H_2, O_2 and CO.

Surface area and Porosity: Determination of surface area. Porosity and pore size distribution. Mercury porosimeter.

Classification of catalysts based on electrical conduction. Adsorption on specific crystal planes; geometric factor in catalysis: Balandin's multiplet theory and Valence angle conservation. Electronic effect in catalysis by metals. Catalysis by semiconductors and solid acids (zeolites etc). Role of diffusion in catalysis.

2. Catalysis in Energy and Environment (16)

Use of fossil fuels and role of catalysts in controlling pollution. Biomass and Synthesis of methanol. FT synthesis. Zeolite catalysts and MTG process. Production of biodiesel. Role of semiconductors and zeolites in auto-exhaust catalysts. CFCs and role of catalysts in their mitigation. Atom economy in catalysis.

3. Kinetics and mechanisms of catalysed reactions (14)

Kinetics of catalysed reactions and rate expressions. Temperature dependence of catalysed reaction rates. Mechanism of catalysed reactions such as hydrogenation of ethene, oxidation of CO, decomposition of N_2O, decomposition of isopropanol.

4. Electrocatalysis (14)

Basic electrocatalytic concepts, comparison of electrocatalysts, Electrosorption. Porous gas diffusion electrodes. Electrolysis of water and role of electrocatalysts. Hydrogen evolution reaction and investigation of its detailed mechanisms. Choice of electrocatalysts. Oxygen reduction reaction and electro-organic oxidation e.g. methanol. Special features of electro-catalysis. Principles of electrosysnthesis.

5. Preparation of Catalysts (6)

Various methods for preparation of bulk catalysts: Precipitation method, Impregnation method catalyst impregnation with or without interaction between support and catalyst. Synthesis of microporous solids. Synthesis of mesoporous solids.

.6. Thermal and Spectroscopic Methods in Heterogeneous Catalysis (10)

Characterization of the catalysts by temperature programmed desorption using probes such as ammonia and pyridine molecules. Characterization of adsorbed molecules/intermediates by ir spectroscopic techniques. Application of spectroscopic methods such as XPS, EXAFS, EPR, NMR and Moessbauer in characterization.

7. Zeolite Catalysis (8)

Structure building in zeolities such as A, X, Y and ZSM-5, producing Zeolite acidity and Zeolite modification. Nature of active sites and their characterization. Shape Selectivity. Identification of Zeolite structures through modern instrumental techniques, adsorption and acidity measurements.

8. Photocatalysis (6)

Introduction to semi-conductor surface and catalysis. Catalytic reactions on illuminated semi-conductors. Principles of photocatalytic reactions, photocatalytic decomposition of water at semi-conductor electrodes. Solar energy conversion by photochemical process.

9. Case Studies and Review of recent journal articles (20)

cases such as catalytic oxidations, Friedel Crafts Reactions, DeNOx catalysts, decomposition of H_2O_2. Electrocatalysis with Pt-M type catalysts, nanocatalysts employing use of nanoparticles of Au, Ag, Pt etc. Synthesis, characterization and catalytic properties of some well known catalysts such as γ-alumina, ZnO, titania, ZSM-5 etc.

Note : *Topics 1 – 4 and 9 are compulsory. The remaining topics may be discussed along with topic 9 through teaching/project work/assignment/student seminars etc. equivalent to 12 – 16 contact hours. The SEA question paper will carry minimum 25% compulsory numerical problems.*

Text Books:

1. Heterogeneous Catalysis, G. C. Bond
2. Heterogeneous Catalysis: D.K. Chakrabarty and B. Viswanathan,
(New Age International Publishers)

Reference Books and Journals:

1. Catalysis: Principles and Applications
(Eds. B. Viswanathan, S.Sivasanker, A.V.Ramaswamy), Narosa Publishing House)
2. Catalysis: Selected Applications, B. Viswanathan, Narosa Publishing House
3. Introduction to Surface Chemistry and Catalysis, G.A. Somorjai, John Wiley, N.Y
4. Principles and Practice of Heterogeneous Catalysis, J.M. Thomas W.J. Thomas, 1996; VCH, New York.
5.Theoretical Heterogeneous Catalysis, R.A. van Santen, 1991; World Sc, Singapore.
6.Spectroscopy in Catalysis, J.W. Niemantsverdriet, 1995, VCH, New York.
7.The microkinetics of Heterogeneous Catalysis, I.. A. Dumesic and others 1993; American Chemical Society, Washington, D.C.
8.Molecular Sieves, R. Szostak, 1989, Van Nostrand, Reinhold.

CHPO –504: NANOSCIENCE: Concepts and Applications (4 credit)

1. Essential concepts and definitions (6)

1.1 interdisciplinary nature, quantum effects, catalysis, colours from colloidal Gold
1.2 Moore's law
1.3 Biological systems
1.4 Atomic structures: Domains and twinning, Wolf construction Chemical properties: catalysis

2. Electronic and Electrical properties (20)

2.1 Chemistry of solid surfaces 2.2 Zero dimensional systems: nanoparticles
2.3 One dimensional systems: nanowires and nanorods
2.4 Metallic nanowires and quantum conductance.
2.5 Carbon nanotubes and dependence on chirality. Quantum dots
2.6 Two dimensional systems: Thin Films 2.7 Special nanomaterials

3. Fabrication of nanoscale materials: top-down vs bottom-up (12)

3.1 Thin film deposition; Epitaxial growth; CVD, MBE, plasma
3.2 Lithographic; photo, e-beam, Etching, FIB
3.3 Synthesis; Colloidal dispersions 3.4 Atomic and molecular manipulations
3.5 Self assembly Growth modes: Stransky-Krastinov, Ostwald ripening

4. Investigation of important nanomaterials (20)

Silica, Gold, CdSe, Iron oxide, Carbon

5. Characterisation of nanomaterials (12)

5.1 Beam probe methods: TEM, EDX, SEM etc.
5.2 Scanning probe methods: STM, STS, AFM etc
5.3 Other methods: Optical spectroscopy. Light scattering.

6. Applications of nanomaterials (10)

Polymers; DNA and high-information molecules; Drug delivery, Sensors, nanocatalysis, air pollution control.

7. **Laboratory/Project work/Assignment (20)**

7.1 Synthesis of Au or Ag nanocrystals and spectral analysis.
7.2 Optolithography and electron microcopy,
7.3 Atomic force microscopy of nanostructures.
7.4 Synthesis of Nanocomposites, X-ray diffraction.
7.5 Synthesis of nanoporous material and adsorption studies

REFERENCES:

1. L. Cademartiri and G.A.Ozin, Concepts of Nanochemistry, 2009, Wiley-VCH
2. C.N.R. Rao and A. Govindaraj *"Nanotubes and nanowires",2005*(RSC Publ.)
3. G. Cao, *Nanostructures and Nanomaterials, 2004* (Imperial College Press)
   P. Yang (Ed), *The Chemistry of Nanostructured Materials,*2004
   R. Saito, *Physical properties of Carbon Nanotubes,* 2004
   G. Q. Lu(Ed), *Nanoporous Materials: Science and Engineering,*
   J. M. Tour, *Molecular Electronics*, 2004 (Imperial College Press)
4. H. S. Nalwa (Ed), "*Encyclopedia of Nanoscience and Nanotechnology",* (American Scientific Publishers, Los Angeles, 2004).
5. E Roduner, Nanoscopic Materials Size-Dependent Phenomena, RSC Publishing, Cambridge, 2006.
6. G.A. Ozin and A.C. Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials, RSC Publishing, Cambridge, 2005.
7. C.P. Poole and F.J. Owens, Introduction to Nanotechnology, John Wiley and Sons, Singapore, 2003.

CHPO – 505: Lab Course in Applied Chemistry (4 credit)

1. Data Handling and Spreadsheets (20)

i. Statistics for small data sets

ii. Linear least squares – How to plot the right straight line

iii. Exercise pg.111 – 121 Ref. 1

2. Stoichiometric Calculations and acid – base equilibria (20)

Exercise/problems pg. 183 – 187 and pg. 260 – 264 of Ref. 1

3. Spectrochemical Methods (20)

Questions/Exercise and problems pg. 515 – 519 of Ref. 1

Spectral Analysis

4. Chromatographic Separations (20)

a) Column Chromatography

1. Separation of Magnesium or zinc and cadmium by ion exchange chromatography.
2. Separation of fluorescein and methylene blue

(b)Gas Chromatographic Analysis

1. Optimum flow rate for the determination of chloroform using Van Deemter equation.
2. Quantitative analysis of a mixture of chloroform and carbon tetrachloride.

(c) HPLC Analysis.

HPLC analysis of (a) benzaldehyde and benzyl alcohol.
(b) toluene and xylene

(d) Thin Layer Chromatography.

To separate a mixture of Amino acids.

(e) Analysis of given GC – MS spectra (any three)

(The above are illustrative examples. Equivalent alternative experiments may be floated.)

5. Self Study Module (20)

Development of analytical procedures of industrial importance through literature search/ Journal of Chemical Education

Reference Book

1. G. D. Christian, Analytical Chemistry, 6^{th} Ed.

CHPO - 506: Laboratory Course in Physical Chemistry-I (8 Credits)

- This is a course of investigatory type of experiments in various areas of Physical Chemistry. Under each category several modules are identified. Each module is roughly equivalent to 1 Credit or about 5 experiments of 6 hours duration.
- The student will be assigned up to eight modules by the corresponding faculty – in – charge/course coordinator depending upon whether the Department Council who may decide to float the course either as a 4 credit course or a 8 credit course.

A] Adsorption

1. Synthesis of a suitable adsorbent (e.g activated carbon) and its characterization by surface area, iodine value, total acidity and pzc
2. Adsorption of monovalent and divalent metal ions and their mixture on a suitable adsorbent. Applicability of Freundlich and Langmuir Adsorption isotherms.
3. Adsorption characteristics of pollutants such as dyes and/or surfactants on a suitable adsorbent.

B] Electrical Conductivity

1. Synthesis of a n – type semiconductor (e.g ZnO) and measurement of its electrical conductivity at different temperatures
2. Synthesis of a p – type semiconductor (e.g NiO) and measurement of its electrical conductivity at different temperatures.

C] Magnetic measurements.

1. Preparation of compounds such as CuO and Cu_2O and determination of their stoichiometry and comparison of their room temperature magnetic susceptibilities with that of $CuSO_4.5H_2O$
2. Preparation of a metal oxide e.g MnO or MnO_2 and study of their magnetic behaviour at low temperatures.

D] X – Ray Diffraction

1. Preparation of a transition metal oxide (e.g ZnO, NiO) by 3 different precursors and their characterization by chemical analysis and XRD
2. Preparation of apinel oxide (e.g $MgAl_2O_4$ or Mn_3O_4) and their characterization by chemical analysis and XRD

E] Thermal Analysis

1. Study of thermal analysis (TG/DTA/DSC) in atmosphere of evolved gases
   e.g decomposition of $CaCO_3$, $KClO_3$ etc in environment of gases such as N_2, O_2, CO_2)
2. Synthesis and study of thermal decomposition patterns to investigate types of desorbed water, evolution of lattice oxygen and phase transition in a suitable compound.

F] Photocatalysis:

1. Synthesis of a photocatalyst (e.g TiO_2 or ZnO) by two different precursors and study kinetics of photocatalytic degradation of a suitable pollutant.
2 Photocatalytic synthesis of an organic compound
3. Photocatalytic degradation

G] Heterogeneous Catalysis:

1. synthesis of a catalyst e.g ZnO by different methods such as thermal decomposition, precipitation, sol – gel, combustion, freeze drying etc.
2. Identification of acidic and basic sites by temperature programmed desorption
3. Dehydrogenation and dehydration studies of an alcohol in a gas phase catalytic reaction.
4. One pot catalytic synthesis of an organic compound.
5. Kinetics of catalytic decomposition of hydrogen peroxide.
6. Investigation of catalytic methylation of phenol or a similar reaction in liquid or vapour phase and study of product distribution
7. Finding oxidation states of a transition metal oxide by ESR, XPS, chemical analysis, magnetic measurements and from electrode potentials
8. Functionalisation of catalyst surfaces and characterization by ir spectroscopy

H] UV – VIS (DRS)

1. Synthesis of pure and doped semiconducting materials and determination of their absorption edges.
2. Kinetics of crystallization of a solid material.

I] Infra – red spectroscopy:

1. Synthesis of various crystalline modifications of a hydrous transition metal oxide and their characterization by infra – red spectroscopy.
2. Investigating esterification reaction by using solid acid catalyst and study of the reaction kinetics by ir spectroscopy.
3. Study of kinetics of zeolite synthesis by infrared spectroscopy.
4. Identification of acidic and basic sites of a catalyst by insitu infrared spectroscopy.

J] Electrochemistry-I

1. Construction of a Leclanche and/or alkaline manganese battery and study of their discharge characteristics in relation to a commercial product
2. Repairs of an old Lead - Acid battery and determining its state of charge.
3. Construction and Testing of a laboratory mini fuel cell
4. Construction of Tafel Plots for electrolysis of water on various platinised electrodes
5. Investigating the relationship between pH and activity coefficients in different electrolytes
6. Determination of stability constants of coordination compounds by electrochemical method. e.g copper complexes with ligands such as NH_3, N_2H_4 and en.
7. Electroless deposition of a metal on a variety of substrates and finding the charateristics of the deposits.
8. Comparison of throwing power of a metal on given substrates by electroless

deposition and electroplating.

9. Investigating conditions for simultaneous deposition of two metals (e.g Cu and Ag) by electroless plating and/or electroplating.
10. Cyclic voltammetry of F^{2+}/Fe^{3+} redox couple on Pt and modified Pt electrodes.
11. Cyclic voltammetry of dissolved oxygen on Pt and oxide modified electrodes
12. Synthesis of a single crystal solid electrolyte as well as its powdered form such as a proton conducting electrolyte e.g phosphotungstic acid and determination of its ionic conductivity by Electrochemical Impedance Spectroscopy.
13. Study of corrosion of a metal such as Fe and/or Zn in different aqueous media and investigating role of inhibitors.
14. Construction of Pourbaix diagrams for corrosion of Zn and/or Fe
15. Study of corrosion potentials and corrosion current for metals such as Zn, Fe or steel.
16. Determination of electrode potentials in solid mixed valent oxides.
17. Investigating conditions for electrosynthesis of a compound e.g ZnO, aniline, polyaniline

K. Gas Chromatography

1. Separation of alcohols and their mixtures e.g 1 – propanol and 2 - propanol
2. Separation of amines and their mixtures e.g 1 – butanamine and 2 – butanamine (separations to be conducted on specific columns and investigate conditions for optimum resolution of the components)

L. Colloids and Microemulsions

1. preparation of micelles and microemulsions and construction of phase diagrans
2. preparation of mesoporous materials through self assembly of surfactants

M. Green Chemical Processes

1. use of pure and mixed metal oxides or clays or zeolites as solid acids to investigate catalytic reactions e.g reactions such as Fridel Crafts alkylation or acylation reactions, aldol condensations, oxidation of alcohols, Henry reactions etc.
2. catalytic synthesis in supercritical fluids such as CO_2

N. Nanomaterials

1. synthesis of nanoparticles of metals and metal oxides and their characterization by XRD and electron microscopies.
2. synthesis and characterization of carbon nanotubes
3. synthesis of high surface area carbons and to test their suitability as adsorbent or supercapacitor.
4. nanocatalysts for enhanced activity.

O. Computational Chemistry

1. Development and Testing of computer programs (either in BASIC/FORTRAN OR C)
   i. least square fit method and its application to experiments in Physical Chemistry.
   ii. to obtain derivative plot in pH-metry/potentiometry

iii. matrix multiplications and its applications to Group Theory

2. molecul;ar energetics calculations using molecular mechanics and semi – empirical methods (use of ready programs PC – model/ PC – win etc.)

P. Electrochemistry-II

1. The temperature and concentration dependence of decomposition voltage of an aqueous acid solution (HCl or H_2SO_4)
2. Potentiometric measurements of the kinetics of oxidation of oxalic acid.
3. Potentiometric titration of Fe^{2+} with Ce^{4+} .
4. Measurement of electrolytic conversion at electrodes
5. Kinetics of ester saponification by conductance measurements.
6. Tafel plots for H_2 and O_2 evolution
7. Kinetic Investigation with cyclic voltammetry using Fe^{2+} / Fe^{3+} system.
8. Cyclic Voltammetry with microelectrodes
9. Cyclic Voltammetry of organic molecules
10. determination of surface area by chronoamperometric measurements.
11. determination of diffusion coefficient of ferricyanide ion by rotating disk electrode.
12. measurements of short circuit currents of various corrosion cells.
13. Determining electrochemical response of simple and stainless steel by cyclic voltammetry.
14. Testing of a silver ion sensitive electrode
15. Electrogravimmetric determination of copper.
16. Electrochemical iodination of ethanol.

Ref. – Rudolf Holes, Experimental Electrochemistry, Wiley – VCH.

CHPO – 507 Computational Chemistry (2 credit)

1. Introduction to Computers (20)

1.1 Need of computers for chemistry, definition and history of computers.
1.2 Computer Organisation.
1.3 Introduction: computer to hardware and software.
1.4 Representation numbers of (integers and real) and characters, Boolean algebra.
1.5 Programming languages (Low level, High level).
1.3 Problem solving with computers, Algorithm, Flow chart, Editor, Compiler and program.

2. FORTRAN Programming (50)

2.1 Statement (formatted and unformatted).
2.3 Integers and real variable.
2.4 Equations and Statements in FORTRAN, Library functions.
2.5 Branching facilities and control statements.
2.6 Dimensions, One, Two and Three dimensional arrays.
2.7 DATA Equivalence and COMMON statements.
2.8 Subprograms, Functions, (Students may be trained either in Fortran or C programming)

3. Programming for Chemistry (30)

3.1 Problems in Kinetics, Spectroscopy
3.2 Quantum Chemistry and Statistical Thermodynamics.

TEXT BOOKS:

1. Computers and Commonsense, R. Hunt and J. Shelley, Prentice-Hall, New Delhi, (1987).
2. Introduction to FORTRAN-77 and the personal computer, H. Hammond, W.B. Rogers, J.B. Crittenden, McGraw-Hill, New York (1987)
3. Monte Carlo Methods Vol.I: Basics (1986); M.H. Kalos and P.A. Whitlock, John Wiley, New York.

REFERENCE BOOKS:

1. FORTRAN-77 featuring structured programming, L.P. Meissner and E.I. Organick, Addison-Wesley, USA (1984).
2. Computers in Chemistry, K.V. Raman, Tata McGraw-Hill, New Delhi (1993).
3. Numerical Methods and Software, (1989); D. Kahaner, C. Moler and S. Nash., Prentice Hall, Englewood Cliffs.
4. Simulation and the Monte Carlo Method; R.Y. Rubinstein John Wiley, New York.
5. Monte Carlo Simulation in Statistical Physics, (1989)., K. Binder, and D.W. Heermann; Springer Verlag, Heidelberg.

CHPO – 508: Radiation Chemistry (2 credit)

Isotopes and Nuclear Reactions: (20)

Isotopes, isobars and their formation and classification. Separation of isotopes by mass spectrometer. Isotopic separation by gaseous diffusion and chemical exchange methods. Compound Nucleus theory. Classification of nuclear reactions. Nuclear reactions induced by charged particles and neutrons. Artificial radioactivity: principle and applications.

Interactions of Radiation: (20)

Interaction of ionising radiation with matter and quantitative characteristics. Effects of ionising radiation on water, aqueous solutions and organic/inorganic compounds. hydrated electron. Reactions of the water radicals with substrates, Properties of some radicals generated by the reaction of water radicals with substrates. Ultra sound, hydrogen peroxide and reducing agents

Radioisotopes and Applications: (20)

The tracer method. Tautomerism and mechanism of rearrangements and those involving free radical formation., mechanism of oxidation and reduction reactions.

Radioactive tracers and applications of tracer techniques in various chemical investigations, dating, biology and medicine.

Synthesis of Radiolabelled Compounds: (16)

Compounds labelling by C-14, P-32, S-35, I-131. Synthesis by isotope exchange.

Mossbauer Effect: Mossbauer effect, Mossbauer spectroscopy and applications. **(12)**

Radiation dosimetry. Radiation handling and disposal. **(12)**

Reference Books:

1. Essentials of Nuclear Chemistry, H.J.Arnikar,Wiley Eastern Pvt.Ltd., NewDelhi (1990).
2. Nuclear and Radiation chemistry, by B.K. Sharma, G oel Publishing House, Meerut (1997).
3. Nuclear and Radiochemistry, by G. Friedlander, J.W. Kennedy, E.S. Macia and J.M. Miller, John-Wiley and Sons, Inc., New York (1981).
4. Nuclear Chemistry, by U.N. Dash, Sultan Chand and Sons, New Delhi (1991).

CHPO – 509: Applied Electrochemistry (2 credit)

1. Basic Electronics (20)

Introduction to Components: Resistors, Capacitors, charging and discharging condensers, LC and RC circuits, parallel circuits.

Semiconductors: classification of semiconductors on the basis of band theory, intrinsic and extrinsic semicoductors, p-n junctions, basic principles of operations, p-n diode and its applications.

Amplifiers: classification of amplifiers depending on coupling, mode of operation and frequency response.

Differential Amplifiers: basic circuit and principle, operational amplifiers, general applications, inverting and and non-inverting, adder, substractor, integrator and differentiator. Integration to digital computers.

2. Electroanalytical Techniques (20)

Principles and applications of the following techniques:

i. amperometry

ii. cyclic voltammetry

iii.voltammetry at rotating disk electrodes

iv. electrochemical impedance spectroscopy

3. Corrosion (20)

Corrosion and electrochemical kinetics. Mechanism of electrochemicalcorrosion. Mixed electrode and mixed potential. Overpotential and polarization. Current density - potential curves and determination of corrosion current density. Hydrogen and oxygen overpotentials and corrosion. Protective film formation and passivity. Types of electrolytic corrosion and forms of localized corrosion, practical cases of corrosion. Corrosion prevention. Corrosion inhibitors. Corrosion Testing. Polarization tests and impedance spectroscopic measurements.

4. Sensors – Basic Concepts (20)

Introduction to principles of chemical sensing; Signal transduction; Physico-chemical and biological transducers; Sensor types and technologies.

Main technical definitions: calibration, selectivity,

sensitivity, reproducibility, detection limits, response time.

Carbon nanotubes and their derivatization for sensor applications. Chemically modified electrodes

5. Electrochemical Sensors (20)

Electrochemical sensors (amperometric, potentiometric, conductometric); Semiconductor transducers (ISFET, ENFET);

Sensor Engineering and applications

Methods for sensors fabrication: self-assembled monolayers, screen printing,

photolithography, microcontact printing, MEMS. Engineering concepts for mass production. Environmental monitoring, Test-strips for glucose monitoring.

Textbooks

1 Jiri Janata, Principles of Chemical Sensors, Plenum Press, 1990
2 J.O.M. Bockris and A.K.N. Reddy,Modern Electrochemistry: by Vol. 1, 2 and 3, Plenum, New York
3 A. J. Bard, L. R. Faulkner, Electrochemical Methods

Other Reference Books and Material:

1. Principles of Chemical and Biological Sensors, D. Diamond Editor, John Wiley and Sons, 2000.
2. Chemical Sensors and Biosensors, Brian Eggins, John Willey and Sons, 2002.
3. Sensors, Nanoscience, Biomedical Engineering, and Instruments. Richard Dorf Editor, CRC Taylor and Francis, 2006.
4. Optical Biosensors. Present and Future. Editors: F. Ligler, C. Rowe Taitt, Elsevier, 2002.
5. Introduction to Bioanalytical Sensors, Alice Cunningham, John Wileyand Sons, 1998.
6. Chemical Sensors and Biosensors for Medical and Biological Applications, Ursula Spichiger-Keller,Wiley-VCH, 1998.

Review articles:

1. Electrochemical Sensors, Eric Bakker, Anal. Chem. 2004, 76, 3285-3298.
2. The New Wave of Ion-Selective Electrodes, E. Bakker and E. Pretsch, Analytical Chemistry, 74, August 2, 2002, pp. 420A-426A.
3. Centennial Retrospective on Chemical Sensors, Jiri Janata. Analytical Chemistry, 73, March 1, 2001; pp. 150 A -153 A.

CHPO – 510: Biophysical Chemistry (2 credit)

1. Biological Cell and Bioenergetics (16)

Structure of biological cell and functions of proteins, enzymes, DNA and RNA in living systems.Helix coil transition

Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP and its synthesis from ADP.

2. Statistical mechanics and biopolymer interactions (32)

Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structures.

Polypeptide and protein structures, introduction to protein folding problem.

Forces involved in biopolymers. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions.multiple equilibria and various types of binding processes in biological systems.

3. Thermodynamics of biopolymer solutions and their molecular weights (32)

Thermodynamics, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system. Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions

4. Cell membrane and transport of ions. (20)

Strucuture and functions of cell membrane, ion transport through cell membrane. Irreversible thermodynamic treatment of membrane transport. Nerve conduction.

Reference Books

1. A. L. Lehninger, Principles of Biochemistry, Worth Publishers
2. L. Styrer, W. H Freeman
3. Voet and Voet,Biochemistry, John Wiley.
4. H. Dugas and C. Penny, Bioorganic Chemistry- A chemical approach to enzyme action Springer – Verlag.
5. F. Wold, Macromolecules: Structure and Functions, Prentice Hall

CHGO – 501: Biological Chemistry **(2 credit)**

1. Basic Concepts: **(25)**

Biological cell, Structure of biomembranes. Structure and functions of proteins, enzymes, DNA, RNA in living systems.

Role of metal ions in biological systems, Na+/K+ pump

Bioenergetics and ATP cycle.

Biological redox reactions

2. Biopolymers: **(25)**

Statistical Mechanics in Biopolymers, Biopolymer Interactions, Thermodynamics of Biopolymer Solutions, Cell membrane and Transport of Ions

3. Enzymes: **(25)**

Properties of enzymes – catalytic power, specificity and regulations

Nomenclature, classification, extraction, purification. Identification of active sites.

Mechanism of enzyme action and role of coenzymes.

Kinetics of enzyme catalyzed reactions

4. Applications: **(25)**

Laboratory Experiments/Project work/ Seminars with respect to specific applications in Inorganic/Organic/Physical Chemistry, biotechnology.

This may include

- structure determination by XRD, NMR, ESR and optical properties
- biocatalysis, drug design, drug delivery
- pharmacokinetics

Reference Books:

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, (University Science Books)
2. H. Dugas and C. Penny, Biorganic Chemistry: A chemical approach to enzyme action (Springer – Verlag)
3. D. Voet, J. G. Voet and Pratt, Fundamentals of Biochemistry 2002. (J. Wiley N. Y.)
4. I. Tinoco, K. Sauer, J.C. Wang, and J.D. Puglisi, Physical Chemistry: Principles and Applications in Biological Sciences, 4th Edition (2002).
5. C.R. Cantor and P.R.Schimmel: Biophysical Chemistry, Part I: The Conformation of Biological Macromolecules, Part II, Techniques for the study of biological structure and function, (Freeman and Co, 1st ed., 1980.)
6. P. Atkins and J Paula, Physical Chemistry for the Life Sciences (2006
7. David G. Nicholls and Stuart J. Ferguson: Bioenergetics (Academic Press 2002.)

CHGO – 502: GREEN CHEMICAL PROCESSES (2 credits)

1. Principles of Green Chemistry (**12**)
Evaluating the Effects of Chemistry
Evaluating Feedstocks, Starting Materials,
Reaction Types; Methods to Design Safer Chemicals, and Future Trends

2. Toxic Heavy Metal Ions: the Problem (**12**)

3. Solid Catalysts and Reagents: (**12**)
Inorganic Supports; Ion-exchange

4. Solid Acids and Bases, Zirconia and Metal Oxides, (**32**)
Clays and Heteropolyacids

5. Working without Organic Solvents (**12**)
Solventless Reactions and Reactions in Water

6. Microwaves and Fluorous Solvents (**20**)
Alternative Solvents: Ionic Liquids
Supercritical CO_2

7. Experimental assignment

Textbooks:

1) *Green Chemistry: Theory and Practice*, by Paul T. Anastas and John C. Warner
2) *Introduction to Green Chemistry*, by Albert S. Matlack. New York: Marcel Dekker
3) *Organic Chemistry Laboratory: Standard and Microscale Experiments*; Bell, C.E.; Clark, A.K.; Taber, D.F.; Rodig, O.R Saunders College Publishing: Philadelphia

Note: an experimental assignment could be given in lieu of any of the above topics of equivalent weightage

CHGO – 503: Chromatographic Methods (2 credits)

Principles of chromatographic separations: (**12**)
retention, band spreading, resolution
Basic mass transfer equations. **(12)**
System design and column packing techniques.
Fundamentals of Adsorption: (**20**)
Gibbs adsorption Isotherm.
Adsorption Models. Local Equilibrium Theory and solute movement plots.
Liquid Chromatography: **(20)**
Basic components of HPLC, Principles of HPLC,
Stationary phases, sample injection system, columns, detectors.
HPLC method development.
Principles of LC – MS.
Analysis by size exclusion and ion-exchange chromatography.
Ion chromatography.TLC.
Electrophoresis. **(36)**
Priciples of instrumentation, separation and resolution. Gel Electrophoresis. Electrophoresis: electrophoretic migration, capillary electrophoresis, electro-osmotic flow, BB behavior and separation optimization. Capillary electrophoresis – state-of-the-art: Theory vs. Experiment,SDS-PAGE for protein separations: separation mechanism and data analysis; DNA sequencing
Size Exclusion Chromatography: stationary phase design and separation mechanism, theory, data, and data analysis for molecular weight determination

Reference Books:

1. Analytical Chemistry, G. D. Christian (from 6th Ed), John Wiley and Sons, NY
2. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West and F. J. Holler, Harcourt College Publishers, Harcourt Asia PTE Ltd., Singapore.
3. Principles and Practice of Analytical Chemistry, F. W. Fifield and D. Kealey, Blackwell Science Ltd., Kundli, India
4. Analytical Chemistry – Principles and Techniques, L. G. Hargis, Prentice Hall.
5. Analytical Chemistry – Principles, J. H. Kennedy, W. B. Saunders.

CHGO-504: Conventional and Non–Conventional Energy (2 Credit)

1. Introduction to energy and environment (8)

General introduction to various conventional and non conventional energy sources and their utilization. Units of energy.

2. Chemical Energy Sources (40)

2.1 Methods of producing hydrogen, Hydrogen storage and utilization.

2.2 Principles of electrochemical energy conversion,

(a) Fuel Cells: classification and types of fuel cells, conversion efficiency and applications of fuel cells. Solid Oxide Fuel Cells.

(b) Batteries: principles and classification. Lead-acid battery. High temperature batteries. Lithium Batteries

2.3 Coal, Natural gas and Oil

3. Nuclear Energy (20)

3.1 Fast breeder reactors,

3.2 thermonuclear fusion, prototype fusion reactor and advantages of nuclear fusion.

4. Non Conventional Energy (32)

4.1 Solar Energy: Solar radiation and its measurement. Solar energy storage. Photo-electrochemical and Photovoltaic Solar energy conversion. Applications of solar energy.

4.2 Ocean Energy: Principles of ocean thermal energy conversion. Energy from ocean waves and tides

4.3 Biomass as source of energy. Methods of obtaining energy from Biomass

4.4 Generation and storage of energy from wind and waves. Efficiency in energy production.

REFERENCE BOOKS:

1. G. D. Rai, Non-conventional Energy Sources
2. Publications of Tata Energy Research Institutes, New Delhi, Tide and Terinis.
3. R. I. Murray, Nuclear Energy, Pergamon Press Inc
4. C. A. Vincent, Modern Batteries
5. R. Narayan and B. Viswanathan, Chemical and Electrochemical Energy Systems, University Press (India) Pvt. Ltd. (2008)