FACULTY OF APPLIED SCIENCES

SYLLABUS

FOR

M.Sc. CHEMISTRY

(SEMESTER: I-IV)

(Under Credit Based Continuous Evaluation Grading System)

Examinations: 2015-onwards

I K Gujral PUNJAB TECHNICAL UNIVERSITY KAPURTHALA

M.Sc. Applied Chemistry (*Under Credit Based Continuous Evaluation Grading System*)

Semester-I

Sr. No.	Code	Theory Papers	Hours	credits
1	CHL401	Basic Inorganic Chemistry	45	3-0-0
2	CHL402	Reactive Intermediates-I	45	3-0-0
3	CHL403	Physical Chemistry-I (Thermodynamics and Electrochemistry)	45	3-0-0
4.	CHL404	Organic Spectroscopy	45	3-0-0
5.	CHL405	Human Physiology(CHL-405H)-for non-medical Background /Mathematics (CHL-405M)-For Medical background	45	3-0-0
6.	CHL406	Environmental Sciences	30	2-0-0
6	CHP407	Inorganic Chemistry	90	0-0-3
7.	CHP408	Organic Synthesis	90	0-0-3

Theory 17 credits; Practical 6 credits

Semester-II

Sr. No.	Code	Theory Papers	Hours	credits
1	CHL411	Advanced Inorganic Chemistry	45	3-0-0
2	CHL412	Reactive Intermediates-II	45	3-0-0
3	CHL413	Physical Chemistry-II (quantum and statistical Chemistry)	45	3-0-0
4.	CHL414	Advanced Characterization Techniques	45	3-0-0
5.	CHL415	Electrochemical Techniques	45	3-0-0
6.	CHL416	Chemistry of Materials (416-A)/ Pharmacology (416-B)	45	3-0-0
7.	CHP417	Analytical and Electrochemical Techniques	90	0-0-3
8	CHP418	Physical Chemistry	90	0-0-3

Theory 18 credits; Practical 6 credits

Semester-III				
Sr. No.	**Code**	**Theory Papers**	**Hours**	**credits**
1	CHL501	Photochemistry and Pericyclic Reactions	45	3-0-0
2	CHL502	Biophysical Chemistry	45	3-0-0
3	CHL503	Self- Assembled Materials (503A)/ Medicinal Chemistry-I(503B)	45	3-0-0
4.	CHL504	Connection and Disconnection Approach in Organic Synthesis	45	3-0-0
5.	CHL505	Chromatography and Separation Techniques	45	3-0-0
6.	CHL506	Computer for chemist	30	1-0-1
7.	CHP 507	BioPhysical Chemistry	90	0-0-3
8	CHP 508	Multi-step Organic Syntheses	90	0-0-3
Theory 16 credits; Practical 7credits				

Semester-IV				
Sr. No.	**Code**	Theory Papers	**Hours**	**credits**
1	CHL511	Advanced Organic Chemistry	45	3-0-0
2	CHL512	Functional Materials(512-A)/ Medicinal Chemistry-II (512-B)	45	3-0-0
4.	CHP513	Dissertation		0-0-18
Theory 6 credits; Practical 18 credits				

Basic Inorganic Chemistry

CHL401

Credits: 3-0-0

SECTION-I

UNIT-l **12Hrs**

Transition Metal Chemistry: Coordination complexes, ligands and their classification, chelation and chelate.effect, Werners coordination theory, nomenclature, stability of complex and stability constants, stereochemistry, isomerism, Valence bond theory: postulates, examples of complexes, shortcomings.

Coordination Chemistry: Crystal Field Theory d-orbital by electrostatic field (octahedral, tetrahedral and square planar geometry), and magnetic properties (high spin and low spin complexes); factors affecting crystal field. splitting energy (10 Dq value) and spectrochemical series; Structural and thermodynamic effects of d- orbital splitting,(variation of ionic radii, Jahn-Teller effect, hydration and lattice energies of first row transition metal ions), octahedral vs. tetrahedral coordination. Molecular orbital theory for octahedral complexes and Tetrahedral complexes.

SECTION-II

UNIT-2 **12Hrs**

Solid State Chemistry: Determination of points groups; types of close packing, packing efficiency, radius ratio, polyhedral discretion of solids, structure type: NaCI, ZnS, wurtzite, rutile and Cs20, perovskite, spinels. Methods for crystal growth. Electrical properties of materials: semiconductors, Hall effect. Defects in crystals, Color Centres. Luminescence properties of inorganic materials and Quantum dots.

Metal Clusters: Preparation, structure and properties of: Boranes, Diboranes, Carboranes, Borrazincs. Geometric and electronic structure, three, four and higher connect clusters, the closo-, nido-, arachno-borane structural paradigm, Wade rules. Metal carbonyl cluster, heteronuclear cluster, capping rules, isolobal , relationships.

UNIT-3 **15Hrs**

Magnetochemistry of Inorganic Compounds: Explanations of diamagnetism, paramagnetism, ferromagnetism and antiferromagnetism, origin of paramagnetic moment: electron spin moment, and orbital angular moment, magnetic susceptibility, Curie law, Curie-Weiss law, Bohr Magneton, magnetic susceptibility measurement using Gouy and Faraday methods explanation of magnetic behaviours of the following: $K_4[Fe(CN)_6]$, $K_3[Fe(CN)_6]$, $K_2[Ni(CN)_4]$, $K_3[CoF_6]$, $K_3[Mnf_6]$, $Ni(CO)_4$.

SECTION-III

UNIT-3

Nuclear Chemistry: Detection and measurement of radioactivity (G.M. Counter method); Decay kinetics-first order rate equation for radioactive disintegration; Theory of Radioactive disintegration; Radioactive series- Uranium; magic number concept; uses of radioactive and non-radioactive isotopes; transmutation of elements; purity and strength of radio isotopes, Radio chemical principle in the use of Tracers. Size of Nucleus; nuclear forces; nuclear binding energy. Basic principles and types of nuclear reactors; atomic energy and Q values elf nuclear reactions.

UNIT-4 **7Hrs**

Inorganic Reaction Mechanism: Lability and inertness of metal complexes, Factors effecting reaction rate, Substitution reactions in octahedral complexes, types of intermediate formed in substitution reactions, Details of mechanism of hydrolysis (under acidic and basic condition) and the stereochemistry of intermediate formed, Trans effect and their theories, oxidation-reduction reactions, Outersphere and inner sphere reactions. Mechanism of electron transfer reaction.

Books Suggested:

1. Inorganic Chemestry Principales of Structure and Reactivity by James E. Huheey, Pearson; Fourth edition
2. Advanced Inorganic Chemistry by Cotton, Wilkinson, Murillo and Bochmann, Wiley; Sixth edition
3. Concise Inorganic Chemistry by J.D. Lee, Oxford; Fifth edition
4. Inorganic Chemistry, by Duward Shriver, Peter Atkins, W. H. Freeman; 3rd edition
5. R.S. Drago, Physical Methods in inorganic Chemistry, Affiliated East-West Press (Section 1& 2) 2nd Edition, Reinhold New York (1968)
6. H.B. Gray, Electrons and Chemical Bonding. (Section 2), W.A. Benjamin, London (1965).
7. A.B.P. Lever, Inorganic Electronic-Spectroscopy, 2nd Edition
8. Modern Aspects of Inorganic Chemistry; H. J . Emeleus and Sharpe .
9. N.N. Greenwood and A. Earnshaw Chemistry of Elements, Pergamon Press, (Section7) (1984)

CHL402

Reactive Intermediate-I

Credits: 3-0-0

SECTION-I

1. Reaction Mechanism: Structure and Reactivity 12Hrs

1.1 Reactive intermediates:- Formation and stability of Carbocations, Carbanions, Free Radicals, Carbenes, Nitrenes, and Arynes

1.2 Aromaticity: Huckel's rule and Concept of Aromaticity, Annulences and Heteroannulenes, Fullerenes (C60)

1.3 Reaction Mechanism: Structure and Reactivity:-

Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, transition states and intermediates, methods of determiningmechanisms, isotope effects. The Hammett equation and linear free energy relationship, substituent and reaction constants,Taft equation.

SECTION-II

2. Aliphatic Nucleophilic Substitution: **10Hrs**

Introduction, SN 1 and SN 2 Mechanism and evidence, Nucleophilic Substitution of allylic systems Nucleophilic displacements at Allylic halides/tosylates, Nucleophilic Substitution at Benzylic position, Nucleophilic Substitution of allylic, aliphatic trigonal and a vinylic carbon., & Aryl halide, Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements Ambient Nucleophiles, SET Mechanism, Neighboring Group Participation reaction (NGP). The S_Ni mechanisum, Mixed SN 1 & SN 2 Reactions, Effect of substrate structure, attacking nucleophile, leaving group and reaction medium in SN 1 and SN 2 reactions , phasetransfer catalysis, ambident nucleophile, regioselectivity.

3. Aliphatic Electrophilic Substitutions 5Hrs

Introduction, Different mechanism for aliphatic electrophilic substitution (*Bimolecular mechanisms- SE2 and SEi The SE1* mechanism), Electrophilic Substitution accompanied by double bond shift, Aliphatic Electrophilic Substitution in relation to substrate structure, Leaving group & solvent polarity, Effect of substrates, leaving group and the solvent polarity on the reactivity,

SECTION-III

4. Aromatic Nucleophilic Substitution 5 Hrs

Introduction Different Addition –elimination mechanism (SNAr, SN1, benzyne an SRN1 Mechanisms),effect of substrate structure,leaving group and attacking nucleophile,Von Richter, Sommelet-Hauser, and Smiles rearrangements.

5. Aromatic electrophilic substitution 7 Hrs

The arenium ion mechanism, orientation and reactivity in mono substitution and disubstituted aromatics, energy profile diagram, the ortho/para ratio, ipso attack, orientation in different ring systems, quantitative treatment of reactivity in substrates and electrophiles, Diazo coupling, Vilsmeir reaction, Gatterman-Koch reaction, Bechmann reaction,Hoben-Hoesch reaction.

6. Free Radical Reactions 6 Hrs

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatics substrates at a bridgehead, Reactvity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, autooxidation,coupling of alkynes and arylation of aromatic compounds by diazonium salts.Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Books:

1. Organic Reaction Mechanism by Jerry March, John Wiley Ed. 5, 2002.
2. Advanced Organic Chemistry by Francis Carey, Vol. A and Vol. B

CHL-403
Physical Chemistry-I

Credits: 3-0-0

SECTION-I

1. **Classical Thermodynamics**:Brief introduction, partial molar properties; partial molar free energy, chemical potential, partial molar volume, partial molar heat content and their significance, Concept of fugacity and determination of fugacity in liquids and gases. Gibbs-Duhem equation, Determination of partial molar volume by method of intercept, Non-ideal solutions, activity and activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, Determination of activity and activity coefficient, ionic strength, Numericals.

2. **Phase rule:** Recapitulation of phase rule and terms involved in it, Three component system: Representation of ternary systems. Partially miscible three liquid systems: a) system composed of three liquid components, one partially miscible pairs, two partially miscible, three partially miscible pairs, b) system composed of two solid and a liquid components – formation of eutecfic systems, crystallization of pure components only, formation of binary compounds, one double salt formation, formation of binary compounds hydrate 5 formation, formation of ternary compounds, formation of solid solutions, partially miscibility of phases.

SECTION-II

3. **Chemical Dynamics:** Collision theory, modified collision theory, weakness of the collision theory, theory of absolute reaction rates, equilibrium hypothesis, Derivation of the rate equation, statiscal mechanical derivation and thermodynamic formulation. Isotope effect on reaction rate. Primary salt effect, secondary salt effect. Dynamics of uni-molecular reactions, Lindmann, Hinschelwood, KRR and slater's treatment for uni-molecular reactions. Kinetics of fast reactions, study of fast reactions by stopped flow method, relaxation method, flash photolysis and NMR method. Reactions in solution: Reaction between ions, influence of solvent-double sphere model, single sphere model, influence of ionic strength, numerical

SECTION-III

4. **Electrochemistry**: Anomaly of strong electrolytes, Debye-Huckel theory, on sager equation and its verification wien effect, Dhy-Hkenhagen effect, ion solvent, interactions. Thermodynamics of electrifield interface equation, Derivation of electrocapillary, lippmann equation. Structure of electrifield interfaces equation, Electrical double layer, Theories of

structure of electrical double layer. Helmoholtz perrin. Gony-Chapman theory, sternis theory. Polarography: Ilkovic equation and its derivation, concentration polarization, instrumentation, advantages of DME, half wave potential, Applications of polarography. Numericals.

Books Recommended:

1. Physical Chemistry P.W. Atkins.
2. Thermodynamics for Chemists by S. Glasstone.
3. Chemical kinetics K.J. Laidler.
4. Principles of Physical Chemistry, S.H. Maron & C.F. Prutton.
5. Introduction to the Thermodynamics of Biological Processes by D. Jou & J. E. LLebot.

CHL404

Organic Spectroscopy

Credits: 3-0-0

SECTION-I

General Features of Spectroscopy

Introduction to spectroscopy, Nature of radiation, Energies corresponding to various kinds of radiation, Experimental techniques, intensities of spectral lines, Selection rules and transition moments, Line widths, Broadening

Nuclear Magnetic Resonance Spectroscopy:

PMR: Natural abundance of 13C, 19F and 31P nuclei; The spinning nucleus, effect ofexternal magnetic field, precessional motion and frequency, Energy transitions, Chemicalshift and its measurements. Factors influencing chemical shift, anisotropic effect;Integrals of protons, proton exchange, spin-spin coupling- splitting theory, one, two andthree bond coupling, virtual, long range and allylic coupling, magnitude of coupling constant; factors affecting the coupling constant, Chemical and magnetic equivalence,First and second order spectra, A2, AB, AX, AB2, AX2, A2B2 and A2X2 spin systems, Simplification of complex spectra (solvent effect, field effect, double resonance andlanthanide shift reagents).

SECTION-II

Nuclear Magnetic Resonance Spectroscopy:

CW and FT NMR, Relaxation processes, T1 and T2measurements, Applications of PMR in structural elucidation of simple and complex compounds.

13C-NMR: Resolution and multiplicity of 13C NMR, 1H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE and originof nuclear overhauser effect. off-resonance, proton decoupling, Structural applications of13C-NMR., pulse sequences, pulse widths, spins and magnetization vectors, DEPT,INEPT, Introduction to 2D-NMR, COSY, NOESY, HMBC and HSQC spectra

Mass Spectroscopy:

Introduction, methods of ionization EI & CI, Brief description of LD, FAB, SIMS, FD etc., Ion analysis methods (in brief), isotope abundance, Metastable ions, general rules predicting the fragmentation patterns.

SECTION-III

Mass Spectroscopy:

Nitrogen rule, determination of molecular ion peak, index of H eficiency, fragmentation patterns for aliphatic compounds, amines, aldehydes, Ketons, esters, amides, nitriles, carboxylic acids ethers, aromatic compoundsetc.

UV and Visible Spectroscopy of organic molecules:

Measurement techniques, Beer – Lambert's Law, molar extinction coefficient, oscillatorstrength and intensity of the electronic transition, Frank Condon Principle, Ground andfirst excited electronic states of diatomic molecules, relationship of potential energycurves to electronic spectra, Chromophores, auxochromes, blue shift, red shift, hypo andhyperchromic effect, σ-σ*, π-π*, n-π* transitions in organic molecules, Woodward rulesfor conjugated dienes and α, β- unsaturated carbonyl groups, extended conjugation andaromatic sterically hindered systems, Quantitative applications.

Books Recommended:

1. Pavia, Lampman & Kriz, Introduction to Spectroscopy.
2. C.N Banwell "Fundamentals of Molecular Spectroscopy".
3. R. M. Silverstein, G.C.Bassler, T.C. Morrill, "Spectrometic Identification of Organic Compounds.
4. W. Kemp, "Organic Spectroscopy".
5. D.H. Williams, I. Fleming, "Spectroscopic Methods in Organic Chemistry".
6. D.H. Williams, I. Fleming, "Spectroscopic Problems in Organic Chemistry", 1967.
7. R.C. Banks, E.R. Matjeka, G. Mercer, "Introductory Problems in Spectroscopy", 1980.
8. G.M. Barrow "Introduction to Molecular Spectroscopy".

CHL405-H

Human Physiology

Credits :-3-0-0

SECTION-I

1. **Introduction** : Definition and scope of anatomy, physiology and related sciences. (2 lectures)

2. **Cellular Basis of Physiology:** Structure and functions of subcellular organelles, structure and molecular mechanism of skeletal, smooth and cardiac muscle contraction, physiology of membrane transport and cell division (4)

3. **Digestive System:** Physiological anatomy of the digestive system, movements and secretions of its different parts and gut reflexes, digestion of various foods, physiology of gastrointestinal absorption, peptic ulcer, hepatitis, inflammatory bowel disease (4 lectures)

4 **Cardiovascular System**: physiological anatomy of cardiovascular sytem. Origin and spread of cardiac excitation. Cardiac contractibility and its regulation. Cardiac cycle, heart sounds, basic principles of electrocardiogram, cardiac output, venous return and their regulation, Blood pressure and its regulation(4 lectures)

SECTION-II

5.**Respiratory System:** Anatomy of respiratory system , mechanism of pulmonary ventilation , pulmonary volumes and capacities, physical principles and mechanisms of gaseous exchange and transport, regulation of respiration (4 lectures)

6. **Excretory System:** Physiological anatomy of the kidneys and urinary tract, urine formation (glomerular filtration, tubular reabsorption and secretion) and its regulation,. (3 lectures)

7. Endocrinology and Reproduction : **Introduction to and General Mechanisms of physiological action of** Pituitary hormones,thyroid hormones, adrenocortical hormones,Pancreatic hormones ,Parathromone and calcitonin, gonadal hormones(7 lectures)

SECTION-III

8 **Sensory Organs:** Brief anatomical description of sensory organs and Physiology of Vision, Hearing and Pain sensation (3 Lectures)

9 **CentralNervous System**: Structure, impulse generation and conduction in neuron. Anatomy, electrical events and chemical transmission in neuro-effector junction. Anatomy and function of various parts of central nervous system. Physiology of motor control,hunger, thirst, and body temperature.Anatomy and function of limbic system.Physiology of learning, memory and speech.Physiology of consciousness and sleep.(10 lectures)

10 **Autonomic Nervous System:** Anatomical organization , neurotransmitters , adrenergic and cholinergic receptors and responses of effector organs to autonomic nerve impulses.(4 lectures)

BOOKS RECOMMENDED

1. Ross and Willson Anatomy and Physiology in Health and Disease 12th Edition (1 May 2014)
2. Guyton, A.C. & Hall, J.E. Textbook of Medical Physiology. 9th edition, Prism Book Pvt Ltd. India 1996
3. Tortora, G.J. and Grabowski, S.R. Principles of Anatomy and Physiology. 8th edition Collins College Publishers, Luciano, New York.
4. Ganong, W.F. Review of Medical Physiology, 18th edition Appleton and lange, Stanford, USA, 1997

PAPER V

CH-405 (a) Mathematics for Chemists **30 Hrs (1 Hr/week)**

(For students without Mathematics in B.Sc.)

Note: This paper should be taught before teaching papers 403 and 404

SECTION-I

I Vectors and Matrix Algebra 10 Hrs

A Vectors

Vectors, dot, cross and triple products etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem etc.

B. Matrix Algebra

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, skew-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence.

Introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants (examples from Hückel theory).

Introduction to tensors; polarizability and magnetic susceptibility as examples.

SECTION-II

II Differential Calculus 10 Hrs

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc), exact and inexact differentials with their applications to thermodynamic properties.

Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. Reduction formulae, applications of integral calculus.

Functions of several variables, partial differentiation, co-ordinate transformations (e.g. cartesian to spherical polar), curve sketching.

SECTION-III

III Elementary Differential Equations 7 Hrs

Variables-separable and exact first-order differential equations, homogeneous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. Solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and Legendre equation etc., spherical harmonics, second order differential equations and their solutions.

IV Permutation and Probability 3 Hrs

Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples from the kinetic theory of gases etc., curve fitting (including least squares fit etc.) with a general polynomial fit.

Books Suggested

1. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
2. Mathematics for Chemistry, Doggett and Sutcliffe, Longman.
3. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
4. Chemical Mathematics, D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.

Environmental Sciences- CHL406

Syllabus As per UGC

SECTION-I

I Environment — 8 Hrs

Introduction.Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Biodistribution of elements.

II Hydrosphere — 12 Hrs

Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. Hydrological cycle.

Aquatic pollution – inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards.

Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand.

Purification and treatment of water.

SECTION-II

III Soils — 6 Hrs

Composition, micro and macro nutrients, Pollution – fertilizers, pesticides, plastics and metals. Waste treatment.

IV Atmosphere — 8 Hrs

Chemical composition of atmosphere – particles, ions and radicals and their formation.

Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry.

Analytical methods for measuring air pollutants. Continuous monitoring instruments.

SECTION-III

V Industrial Pollution **12 Hrs**

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

VI Environmental Toxicology **14 Hrs**

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes.

Bhopal gas tragedy, Chernobyl, Three mile island, Sewozo and Minamata disasters.

Books Suggested

Environmental Chemistry, S. E. Manahan, Lewis Publishers.

Environmental Chemistry, Sharma & Kaur, Krishna Publishers.

Environmental Chemistry, A. K. De, Wiley Eastern.

Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern

Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.

Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.

Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.

Environmental Chemistry, C. Baird, W. H. Freeman.

CHP-407
Inorganic Chemistry

Inorganic Synthesis

1. Synthesis of Tris(Ethylenediamine)Nickel(II) Chloride and estimation of Ni(II).
2. Synthesis of Potassium Trisoxalatoferrate(III) Trihydrate $K_3[Fe(C_2O_4)_3].3H_2O$ and estimation of anion.

Materials Synthesis

3. Synthesis of metal nanoparticles and studies of their photophysical properties.
4. Ligand directed synthesis of Quantum Dots and studies on the influence of surface directing agents.

Separation Techniques

5. To separate the mixture of metal ions using thin layer chromatography.
6. To perform the solvent extraction for the recovery of metal ions from aqueous medium.

Coordination Chemistry

7. Verification of relative position of ligands in spectrochemical series.
8. Calculation of 10Dq for the given metal complexes and assignment of transitions.

Inorganic Spectroscopy

9. Quantative determination of Cu(II) using spectroscopy.
10. Determination of stoichiometry of metal complex using Job plot method.
11. Determination of stoichiometry of metal complex using mole ratio method.
12. Determination of molar extinction coefficient of metal picrates.

CHP-408

Organic Synthesis

Techniques: (At least One Practical of Each Technique)

Crystallization, purification by Sublimation, Distillation, Fractional Distillation , Steam Distillation, Vacuum Distillation, Preparative chromatography Column Chromatography, TLC stains preparation and Thin Layer Chromatography

(Purity would be checked by m. p. and mixed m. p.).

2. Preparation of Derivatives: (Each Derivative of two Compounds) Oxime, 2, 4-DNP, Acetyl, Benzoyl, Semicarbazone, Anilide, Amide, Aryloxyacetic acid.

3. Preparations: Single Stage (Any 15)

i) Cyclohexanone to Adipic acid
ii) Benzophenone to Benzhydral
iii) Anthracene to Anthraquinone
iv) Chlorobenzene to 2,4-Dinitrochlorobenzene
v) 2,4-Dinitrochlorobenzene to 2,4-Dinitrophenol
vi) Acetoacetic ester to 1-Phenyl-3-methyl-5 pyrazolone
vii) Benzaldehyde to Cinnamic acid
viii) 4-Chlorobenzaldehyde to 4-Chlorobenzoic acid + 4-Chlorobenzyl alcohol
ix) Benzene to β-Benzoyl propionic acid
x) Benzaldehyde to Dibenzylidene acetone
xi) p-Aminobenzoic acid to p-Chlorobenzoic acid
xii) N,N-Dimethylaniline to 4-Formyl-N, N-dimethyl aniline
xiii) Benzophenone to Benzpinacol xiv) p-Nitrotoluene to p-Nitrobenzoic acid
xv) Anisole to 2,4-Dinitroanisole
xvi) Phthalic anhydride to phthalimide
xvii) Phthalimide to Anthranilic acid
xviii) Acetanilide to p-Bromoacetanide
xix) p-Bromoacetanide to p-Bromoaniline
xx) m-Dinitrobenzene to m-Nitroaniline

Pattern of Practical Examination

Q - 1. Techniques: Distillation or Column or TLC	25 marks
Q - 2. Preparation / Derivative	25 marks
Q - 3. Interpretation of spectrum	10 marks
Q - 4. Lab Journal	05 marks
Q - 5. Oral	10 marks

References: Vogel's, Practical Organic chemistry.

CHL411

Advanced Inorganic Chemistry

Credits: 3-0-0

SECTION I

UNIT-1 **10Hrs**

Organic Chemistry: 18 electron rule, synthesis, structure, bonding and reactivity of transition metal complexes with olefins, Cyclopantadienyl, Cyclopentadiene, Benzenoid, π-allyl and Enyl System. **Transition metal- carbon bond**: Metal-alkyls, metal-carbenes and metal-carbynes.

Review of reaction involving: oxidative addition, reductive elimination, migratory insertion, hydride elimination, transmetallation , metal carbonyls.

Brief description of Hydroformylation, Olefin metathesis, cross coupling reactions.

UNIT-2 **12Hrs**

Bio-Inorganic Chemistry: Transition elements in biology- their occurrence and function, active site structure and function of metalloroteins and metalloenzymes. O_2 binding properties of heme and non-heme proteins, co-operative effect, Hill coefficient and Bohr effect. Electron transfer proteins, rubridoxin, fereedoxin and cytochromes, Vitamin B_{12} and cytochrome P_{450} and their mechanism of action.

SECTION II

UNIT-2

Metals in medicine: Therapeutic application of *cis*-Platin, radio-isotopes and MRI agents. Toxicity of metal ions, progression of disease state due to metal unbalancing (metal inons as paradox to life)

UNIT-3 **10Hrs**

Catalysis: Turnover number, turnover frequency, homogenous and heterogenous catalysis, asymmetric synthesis using catalysis. Concept of green chemistry, ionic liquids,Quantume dots and metal-organic formworks.

Inorganic Polymers: Types of inorganic polymers: Comparison with organic polymers: Important synthesis structure aspects and application of silicones. Phosphazenes:Uses, Structure and bonding in Tri- and Tetra- Phosphonitrilic halides.

SECTION III

UNIT-4 **13Hrs**

Supramolecular Chemistry: Nature of non-covalent interactions, salvation and hydrophobic effect preorganistaion and complementarity of binding sites. Thermodynamic and kinetic selectivity ,templates effect high dilution synthesis. Crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, siderophore inclusion cpmpounds, molecular clefts and tweezers.

Ion Recognition: Conformational characteristics, chelate ring size effect, donor group and orientation challenge in anion receptor chemistry, contact ion pairs, cascade complex, remote anion and cation binding sites, Dual host salt extraction.

Books Suggested

1. R.S. Drago, Physical Methods in inorganic Chemistry, Affiliated East-West Press (Section 1& 2) 2nd Edition, Reinhold New York (1968).
2. H.B. Gray, Electrons and Chemical Bonding. (Section 2), W.A. Benjamin, London (1965).
3. F.A. Cotton and G.W. Wilkinsonn, Advanced Inorganic Chemistry. John Wiley and Sons, 6th edition, John Wiley New York (1999).
4. J.E. Huheay, Inorganic Chemistry, Principles of Structure and Reactivity, Harper International, SI Edition, 3rd Edition, Harper London (1978).
5. G. Wilkinson (Ed.) Comprehensive Coordination Chemistry Vol. 3 Chapter 23, Pergamon, Pergamon Oxford (1982).
6. N.N. Greenwood and A. Earnshaw Chemistry of Elements, Pergamon Press, (Section7) (1984).
7. Christopher Master, Homogenous Transition metal catalysis (Section 8) (1981).

CHL412

Reactive Intermediate-II

Credits: 3-0-0

SECTION-I

1. Addition to carbon carbon and Carbon-Hetero Multiple Bonds

Mechanism and stereochemical outcome in the addition of electrophile, nucleophile, freeradicals, Hydration of olefins and acetylenes, Hydroboration and its types, hydroxylaions, Michaeal addition, 1, 3 - dipolar additions, Sharpless asymmetric epoxidation,Addition of Grignard reagents, organozinc, organolithium and Gillman reagents to carbonyl and unsaturated carbonyl compounds, Carbenes and their additions to double bonds - Simmon - Smith reaction, Mannich, Stobbe, Darzen, Wittig, Wittig - Horner and Benzoin reactions. Hydrolysis of esters etc,

Stereochemical aspects to be studied wherever applicable.

Section-II

2. Elimination Reactions:

E1, E2 and E1cB mechanism - E1, E2 and E1cB spectrum - Orientation of the double bond - Hoffman and Saytzeff rules - Competition between elimination and substitution. Typical eliminations reactions - dehydration, dehydrohalogenation and dehalogenation. Stereochemistry of E2 eliminations in cyclohexane systems. Mechanism of pyrolytic eliminations. Chugaev and Cope eliminations.

3. Oxidation Reactions and reduction

3.1Oxidation :- Different oxidative processes,Mechanism - study of the following oxidation reactions oxidation of alcohols - use of DMSO in combination with DCC or acetic anhydride in oxidising alcohols - oxidation of methylene to carbonyl, oxidation of aryl methenes - allylic oxidation of olefins, Formation of C=C, C-C bonds by dehydrogenation, dehydrogenation by quinones , SeO_2, $Hg(OAc)_2$ and $Pb(OAc)_4$, Formation of C-C bond in phenol coupling - acetylene coupling-allylic oxidation-oxidation of alcohol, glycols, halides and amines to aldehydes and ketones - Ozonolysis - oxidation of Olefinic double bonds and unsaturated carbonyl compounds-oxidative cleavage of C-C bond.

SECTION-III

3.2Reduction :-

Introduction. Different reductive processes, Hydrocarbons- alkanes, alkenes, alkynes and

aromatic rings, Carbonyl compounds – aldehydes, ketones, acids, ester and nitriles.Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis. Sodium borohydride,sodium cyano borohydride, LAH, disobutyl aluminium hydride, tin hydride, trialkyl tinhydride, trialkyl silanes, alkoxy substituted LAH, DIBAL, diborane, diisoamyl borane,hexyl borane, 9-BBN, isopinocamphenyl and disiopinocamphenyl borane. Reductionreactions with particular emphasis on Wolf-Kishner reduction, Clemensen reduction.

4. Rearrangements

General mechanistic consideration – Types of migration, Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber,Beckmann, Hofman, Curtius, Schmidt, Shapiro reaction, Fries rearrangement, dienone - phenol, Baeyer - Villiger, Wolf, Stevens (in cyclic systems) and Von Richter rearrangements.

Recommended Books

1. Principles of organic synthesis R.O.C. Norman, Chapman and Hall, London. 1980.

2. Structure and Mechanism by E.S. Gould

3. Advanced Organic Chemistry - Part B by Francis A. Carey and Richard J, Sundberg, 3rd Edition 1990.

4. Organic synthesis by Michael Smith.

5. Carbenes, Nitrenes and Arynes by T.L. Gilchrist and C.W. Rees, Thomas Nelson and Sons Ltd., London

6. Some Modern Methods of Organic Synthesis by W Carruthers, III Edition, Cambridge University Press, 1993.

7. Modern Synthetic Reactions by H.O. House, The Benjamin Cummings Publishing Company, London, 1972

8. Advanced organic chemistry, Mc Murray, Thomas Pvt. Ltd.,

CHL-413

Physical Chemistry-II

Credits: 3-0-0

SECTION-I

1. Introduction

An introduction to quantum mechanics; quantum mechanics vs. classical mechanics; wave–particle duality; and uncertainty principle

2. Schrödinger equation

Wave function and interpretation; time-dependent and time-independent Schrödinger equation; and Eigen value problem

3. Quantum mechanics of some simple systems

Free particle; particle in a box; and harmonic oscillator

4. Angular momentum

Rigid rotor; orbital and spin angular momentum; ordinary angular momentum; Eigen functions for angular momentum; Eigen values of angular momentum; operator using ladder operations; addition of angular momenta; spin and antisymmetry; and Pauli exclusion principle

SECTION-II

5. Hydrogen atom

6. Approximate methods

Perturbation theory; variation theorem; linear variation principle; and application of variation method and perturbation to helium

7. Electronic structure of atoms

Electronic configuration; Russel-Saunders terms and coupling schemes; Slater-Condon parameters; Term separation energies of the p^n and d^n configurations; magnetic effects like spin orbit coupling and Zeeman splitting; and introduction to methods of self-consistent virial theorem

8. Molecular orbital theory

Huckel theory of conjugates systems; bond order and charge density calculations; application to ethylene and butadiene, and extended Huckel theory

SECTION-III

9.Statistical mechanics

Concept of distribution; thermodynamic probability and most probable distribution; the ensemble averaging and its postulates; canonical, grand canonical, and microcanonical ensembles; and distribution laws

10. Partition functions

Translational, rotational, vibrational, and electronic vibration function; and application of partition functions

11. Heat capacity

Heat capacity behavior of solids; chemical equibria and equilibrium constant in terms of partition funtions; Fermi-Dirac statistics; distribution law and applications to metal; and Bose-Einstein statistics

Recommended books

- *Quantum Chemistry*, I. N. Levine, Prentice Hall
- *Introduction to Modern Statistical Mechanics*, David Chandler, Oxford University Press
- *Physical Chemistry*, P.W. Atkins and Julio de Paula, W H Freeman

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CHL414

Advanced Characterization Techniques

Credits: 3-0-0

SECTION-I

1. Modern Methods of Surfaces Analysis **5Hrs**

Scanning electron microscopy: Principle, Specimen Preparation, Replicas Various-application of SEM

2. Transmission electron microscopy **6Hrs**

Instrumentation, Principle, Advantage, Difference between SEM and TEM.

SECTION-II

3. Atomic Force Microscopy **10Hrs**

Principle, Instrumentation, Advantage and disadvantage, scanning force microscopy, shear forces microscopy, lateral force microscopy and magnetic force microscopy.

4. X-Ray diffraction **7Hrs**

Single crystal XRD and powder XRD, Bragg's diffraction law, Unit cell, space group, element of space group, particle size analysis using Scherer formula.

SECTION-III

5. Atomic Absorption Spectroscopy **7Hrs**

General principles, Instrumentation, Hollow cathode lamp, Line width effect in atomic absorption, Cold vapor atomic absorption spectroscopy.

6. Thermo-Analytical Method **10Hrs**

Theory, instrumental requirements and methodology for thermo gravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC), applications

Reference

1. J.Goldstein, D. E. Newbury, D.C. Joy, and C.E. Lym, "Scanning Electron Microscopy and X-ray Microanalysis", 2003.
2. S.L. Flegler, J.W. Heckman and K.L. Klomparens, "Scanning and Transmission Electron Microscopy: A Introduction", WH Freeman & Co, 1993.
3. P.J.Goodhew, J.Humphreys, R.Beanland, "Electron Microscopy and Analysis",
4. Instrumental Methods of Analysis, Willard, Merritt, Dean and Settle, CBS Publisher and Distributors.,1986.
5. Thermal Analysis, W. W. Wendlandt and L. W. Collins, Dowden Hutechin and Ross

CHL415

Electrochemical Techniques

Credits: 3-0-0

SECTION-I

1. Introduction to electrochemistry 15Hrs

Electrode potential, electrochemical cell and its types, Oxidation reduction reaction in electrochemical cell, Half-cell potential, standard hydrogen electrode, calculation of cell potential from electrode potential, Standard Weston cell, The Nernst equation, disproportion and comproportionation. Latimer diagram, Frost diagram, Oxidation reduction titrations

SECTION-II

2. Cyclic voltametry 15Hrs

Electrode used in cyclic voltametry, electrochemical mechanism, E_{ads} mechanism (Adsorbtion mechanism), Butler-volmer equation, Reversible one electron transfer. Linear sweep voltametry, differential pulse voltammetry, Application, Polarography: principle and Application of polarography.

SECTION-III

3. Conductometry 8Hrs

Electrolytic conductance, Measeurement of conductance, Conductometric titration, Application, Oscillometry.

4. Potentiometric methods 7Hrs

Indicator electrode, Instrument for cell potential measurement, Application of potentiometric titration.

References

1. Fundamental of analytical chemistry, Skoog, West, Holler, Crouch, Eighth edition book, 2001.
2. Principles of Instrumental Analysis, Skoog, Holler, Nieman, Fifth edition Thomson Books ,1998.
3. Electrochemical Methods: Fundamentals and Applications, Bard, Allen J.; Larry R. Faulkner, Sencond edition, 2000 Wiley.
4. Handbook of Electrochemistry. Elsevier Science. ISBN 0-444-51958-0. Zoski, Cynthia G. 2007.

CHL416-B

Pharmacology

Credits: 3-0-0

SECTION-I **15Hrs**

General: Introduction to Pharmaceutical sciences, history and development of chemotherapeutic agents, its branches, standards for drugs, naming of drugs, therapeutic index, LD50 and ED50, Pharmaceutical literature, official books, routes of drug administration.

Cell Structure & Cellular Physiology: Subcellular organization, membrane processes, cell metabolism, cell division, Structure and function of epithelial connective, muscular and nervous tissues, Muscle contraction and properties, Nerve impulse generation and transmission. Skull & Skeleton .

Respiratory System: Structure respiratory volumes and capacities, ventilation, compliance and resistance, gaseous exchange and transport in blood, nervous and chemical regulations of respiration. Acid-base balance.

Renal system: Structure of kidney and urinary tract; nephorn transport processes concentration and dilution of urine, renal control of body f luids, plasma clearances, Maturation.

SECTION-II **18Hrs**

Major Categories of formulations, Physical properties and Chemical characteristics of drugs influencing their formulations.

Metrology: Introduction, units of weight and volume in both imperial and metric system, Simple calculations involved in preparing solutions of solids in liquids and liquids based on imperial and metric systems, method of allegation.

Pre formulation considerations: Analytical methods for characterization of drugs, determination of pKa value, pH, solubility profile, and effect of temperature, solution and solid state stability.

Emulsions: Types, identification, and selection of emulgents, preparation and stability. Emphasis may be given on official products.

Suspensions and mixtures: Practical considerations, preparation of products of different categories evaluation, stability, and official suspensions.

Semi-Solid Dosage Forms: A brief description, preparation of ointments, creams jellies and suppositories.

Aerosol Dosage Forms: Advantages, formulation and standardization.

SECTION-III **12Hrs**

Pharmacokinetics: ADME (Absorption, distribution, metabolism- Phase I and Phase II reactions, Excretion) of drugs, important pharmacokinetic parameters- apparent volume of distribution, bioavailability, clearance.

Pharmacodynmics: Elementary idea about drug action, drug targets, neurotransmitters, there ceptor role, Drug Receptor Interactions, types of receptors-ion channel receptors, G-protein couple dreceptors, kinase-linked receptors, ion channels and their control, membrane bound enzymes- activation/deactivation, design of agonists and antagonists.

Principles of toxicology and treatment of poisoning: Introduction, Toxic agents, Toxicity-acute, subacute and chronic, descriptive toxicity tests in animals, General principles of management of poisoning, antidotes, Treatment of heavy metal poisoning and drugs (barbiturates, benzodiazepines, salicylates, morphine & morphine derivatives, alcohol).

Books Recommended:

1. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.

2. B. G. Katzung, Basic and Clinical Pharmacology, Lauge Medical Publication, 1995.

3. Introduction to Pharmacology by P. C. Dandya and S. K. Kulkarni.

CHP-416-A

CHEMISTRY OF MATERIALS

SECTION-I

Interfaces and Liquid Assemblies, Liquid crystal: Nature and structure, Design of liquid crystalline materials, Liquid crystal displays. Inorganic liquid crystals

Spinal molecule: Inverse and normal, Perovskites and related phase, High temperature superconductor

SECTION-II

Thermochromics and photochromic materials

Oxide Glass, Aluminophosphates, Silicates, Endohedral Fullerenes, Nanotubes and Graphene

SECTION-III

Zeolites: Composition and structure, Synthesis, MFI Zeolites in petroleum industry.

Inorganic pigments, Group 14 Semiconductors, Semiconductor system isoelectronic with Silicon. Material used in Light emitting diodes,

Reference

1. Nematic and Cholesteric liquid crystals, P. Oswald, P. Pieranski, Taylor and Francis Group, 2005.
2. Inorganic chemistry, Atkins, Overton, Rourke, Weller, Armstrong, Fifth edition, 2010, oxford.
3. Supramolecular Chemistry. J. W. steed, J. L. Atwood, second edition 2009, Wiely.

CHP417

Analytical and Electrochemical Techniques

Credits: 0-0-3

A. Conductometry

1. Find graphically the equivalent conductance at infinite dilution of weak acid (benzoic acid, succinic acid, acetic acid) and hence determine the thermodynamic dissociation constant of the weak acid.
2. Determine the equivalent conductance of strong electrolytes (KNO_3, KCl) at several concentrations of its aqueous solution and verify the Onsagar's equation.
3. Determine the equivalent conductance at infinite dilution of weak electrolytes (CH_3COOH, NH_4OH) in their aqueous solutions using Kohlraush law.
4. To determine relative strength of monochloroacetic and acetic acid by conductance measurements.

B. Potentiometry and *p*Hmetry

5. To determine the dissociation constant of a dibasic acid (malonic acid)
6. The potentiometric titration of a mixture of Chloride and Iodide with $AgNO_3$.
7. To determine the degree of hydrolysis of aniline hydrochloride and hence hydrolysis constant of the salt.
8. Determination of acid and basic dissociation constants of an amino acid and hence the iso-electric point of the acid.
9. Titration of Phosphoric acid solution with NaOH using quinhydrone electrode.
10. The Potentiometric Determination of Solute Species in a Phosphate Mixture
11. The Potentiometric Titration of Copper with EDTA.

C. Electrogravimetry and Coulometric titrations

12. Determination of Copper and Lead in a given sample of Brass Electrogravimetrically.
13. Determine coulometrically the concentration of Nickel and Cobalt from a given mixture.
14. The coulometric titration of cyclohexene.

D. Polarography and Stripping methods

15. The polarographic Determination of Copper and Zinc in the given sample of Brass.
16. Study the polarographic waves produced by dissolved oxygen.
17. Determine the half wave potential of Cd^{2+}, and Zn^{2+} ions in 0.1 M KCl solution.
18. Plot a polarogram for a mixture of Cd^{2+}, Zn^{2+}, and Mn^{2+}, ions.
19. Determine of formula and the stability constant of complex formation of a metal ion complex.
20. Determine the amount of Copper and Zinc in tap water using DPP.

21. Apply stripping methods to determine the concentration of lead in tap water.

Amperometric titrations:

22. Amperomertic titration of lead solution with potassium dichromate.
23. Amperometric titration of potassium sulphate solution with Lead nitrate solution.
24. Amperometric titration of nickel in solution with dimethyl glyoxime.
25. Determine transport number of silver and nitrate ions by Hittorf's method.

CHP418

Physical Chemistry Lab

- **Error analysis and statistical error analysis**

Errors, types of errors, minimization and distribution of errors; precision, accuracy, and combination; statistical treatment of error analysis; student 't' test; null hypothesis; linear regression analysis; and curve fitting

- **Adsorption**

Adsorption isotherm; and surface tension-concentration relationship for solutions

- **Phase equilibria**

Congruent composition and temperature of a binary system; phase diagram of a three component system; and oscillating reaction

- **Chemical kinetics**

Rate and order of reaction (ester hydrolysis in homogeneous/heterogeneous media and oxidation of iodine with hydrogen peroxide/iodine clock); influence of temperature, concentration of reactant and catalyst, and ionic strength of the media on rate constant; primary salt effect on the kinetic of ionic reaction

- **Solutions**

Molecular weight and activity coefficient of non-volatile and non-electrolyte/electrolyte; degree of dissociation of weak electrolyte (deviation from strong electrolyte); and surface tension and viscosity

- **Polymers**

Viscosity and molecular weight of polymers

- **UV-Vis and fluorescence spectroscopy**

UV-Vis spectra of compounds and λmax; effect of solvents (hypochromic, hyperchromic, hypsochromic, and bathochromic shifts); estimation of molecular extinction coefficients; emission and excitation spectra, effect of solvent; and estimation of quantum yields

- **Electrochemistry**

(a) Conductometry: velocity constant, order of reaction and energy of activation; strength of strong and weak acid; effect of solvent on conductance; activity coefficients of ions (Debye Huckel's limiting law); and solubility product of sparingly soluble salt

(b) Potentiometry:formation constant and stochiometry of a complex potentiometrically; strength of strong and weak acids (potentiometer/pH meter); temperature dependence of EMF of a cell; acid-base titration in non aqueous media (pH meter); activity and activity coefficients of an electrolyte; dissociation constant of acid in organic solvents (DMSO, DMF); and thermodynamic constant G, S, and H for the reaction by emf method

(c) Polarimetry:rate constant and enzyme kinetics for hydrolysis/inversion of sugar

Recommended books

1. *Practical Physical Chemistry*, A M James and F E Prichard, Longman

2. *Findley's Practical Physical Chemistry*, B P Levitt, Longman

2. Experimental Physical Chemistry, R C Das and B Behera, Tata McGraw Hill

Semester-III

CHL501

Photochemistry and Pericyclic Reactions

Credits: 3-0-0

SECTION-I

1. Photochemical Reactions **4 Hrs**

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry

2. Determination of Reaction Mechanism **4 Hrs**

Classification, rate constants and life times of reactive energy states – determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions.Types of photochemical reactions – photo-dissociation, gas-phase photolysis.

3. Photochemistry of Alkenes **6 Hrs**

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

SECTION-II

4. Photochemistry of Carbonyl Compounds **8 Hrs**

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic, β, γ-unsaturated and α,β-unsaturated compounds, Cyclohexadienones.Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

5. Photochemistry of Aromatic Compounds **4 Hrs**

Isomerisations, additions and substitutions

6. Miscellaneous Photochemical Reactions **4 Hrs**

Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction.Singlet molecular oxygen reactions.Photochemical formation of smog.Photodegradation of polymers.Photochemistry of vision.

SECTION-III

7. Pericyclic Reaction **15 Hrs**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions,conrotatory and disrotatorymotions, 4n, 4n+2 and allyl systems.Cycloaddition includingantarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloadditions and cheleotropicreactions.Sigmatropic rearrangements – suprafacial and antarafacialshifts of H, sigmatropic shifts involving carbon moieties, 3,3- and – sigmatropic rearrangements. Claisen, Cope and aze –Cope rearrangement.Fluxional tautomerism.Ene reaction.

Books Suggested

1. Essentials of Molecular Photochemistry by A. Gilbert, J. Baggott, CRC Press, London, UK, (1991).

2. Modern Molecular Photochemistry (MMP) by N. J. Turro, University Press, Menlo Park, CA, 1978.
3. Photochemical Key Steps in Organic Synthesis by J. Mattay and A. Griesbeck, VCH, New York, 1994
4. Photochemistry in Organic Synthesis by J. D. Coyle, Royal society of Chemistry, London, 1986.

CHL502
Biophysical Chemistry

SECTION-I

1.Biomolecules

An introduction to the structure and conformation of proteins, nucleic acids, and other biopolymers

2. Water

Weak interaction in aqueous systems, ionization in weak acids and bases; buffering against pH changes in biological systems; water as reactant; and role of water in maintaining the native structure of biopolymers

SECTION-II

3.Bioenergetics and thermodynamics

Biological energy transformations and the law of thermodynamics; concepts of standard free energy, entropy, enthalpy, and chemical potential changes in biochemicalreactions; relationship between equilibrium constant and standard free energy; the effect of temperature and pH on standard free energy; free energy changes associated with hydrolytic and redox (electron transfer) reactions in biological systems

4. Techniques to study structure and function of biomolecules

An overview of UV-Visible, fluorescence, and circular dichroism (CD) spectroscopy; ultra centrifugation, sedimentation velocity and equilibriumdetermination of molecular weights; Diffraction and light scattering techniques; and nuclear magnetic resonance

SECTION-III

5. Study of the behaviour of biomolecules

Ligand interactions at equilibrium and its kinetics;conformational transitions of polypeptides and proteins: helix-coil transition and reversible protein folding; nucleic acid structural transitions; and membrane equilibria and transport

Recommended books

- *Lehninger Principles of Biochemistry*, D L Nelson and M M Cox, Vth Edition, WH Freeman and Company, NY, 2008
- *Biophysical Chemistry I,* C R Cantor and P R Schimmel, Macmillan
- *Biophysical Chemistry II,* C R Cantor and P R Schimmel, Macmillan
- *Biophysical Chemistry III,* C R Cantor and P R Schimmel, Macmillan

CHL503-B

Medicinal Chemistry-I

Credits: 3-0-0

SECTION-I

1) Introduction to Pharmaceuticals, Historical development, Classification drugs,Nomenclature of Pharmaceuticals & Drug metabolism reactions.

2) Structure, stereochemistry, nomenclature, mode of action, specific clinical applications and structure activity relationships, biosynthesis of naturally occurringcompounds and synthesis of prototypical drugs in each category.(Chemical & Pharmacological) for the following classes of drugs.

3)Hormones: Sex hormones and related compounds (Estrogens, Androgens,Progestational agents, Anabolic steroids, Contraceptives), Adrenal cortexhormones, Thyroid hormones and antithyroid drugs, pancreatic hormones,Hypothalamus hormones.

4)Vitamins: Fat soluble vitamins (A,D,E and K), water soluble vitamins (Folic acid,B12 and C).

SECTION-II

5) Adrenergic and cholinergic drugs (Agonist & antagonists):

6)Cholinergic agents: Autonomic blocking and related drugs, Antispasmodic and antiulcer drugs. Antiparkinsonism drugs.

7) Structure, stereochemistry, nomenclature, mode of action, specific clinical applications and structure activity relationships, biosynthesis of naturally occurring compounds and synthesis of prototypical drugs in each category (Chemical & Pharmacological) for the following classes of drugs.

8)Cardiovascular drugs: Vasodilators, Antihypertensive agents,Antihypercholesterolemic drugs, Antiarrhythmic drugs, Sclerosing agents,Coagulants and anticoagulants, Cardiotonic compounds, Cardiac glycosides &inotrpic agents Synthetic hypoglycemic agents.

9)Diuretics: Osmotic agents, Acidfying salts, Mercurials, Purines and related heterocycles, Sulfonamides, Benzothiadiazene and related compounds,Chlorothiazides and analogs.

SECTION-III

10). Stereochemistry, nomenclature, mode of action, specific clinical applications, structure activity relationships, biosynthesis of naturally occurring compounds and synthesis of prototypical drugs in each category (Chemical &Pharmacological) for the following classes of drugs.

11).General Anaesthetics: Theories of General Anaesthetics, Ethers, Halogenated hydrocarbons, Cyclopropane, Nitrous oxide, Barbiturates, Adjuvants to general anaesthetics, metabolism of volatile anaesthetics.

12).**Local Anaesthetics:** Cocoa alkaloids – Cocaine and Synthetic compounds,Esters, Amides, Miscellaneous anaesthetics.

13). **CNS Active Drugs: CNS Depressants:** Hypnotics and sedatives: Barbiturates,Non barbiturates, Amides and Imides, Bezodiazepines, Aldehydes andderivatives, Methaqualone and other miscellaneous agents. Anticonvulsants Barbiturates, hydantoins, oxazolidinediones, succinmides, benzodiazepines,Thenacemide, Glutethimide

Books Recommended:

1. Wilson and Gisvolds Textbook of Organic Medicinal and Pharmaceuticals Chemistry, 8th edition, edited by R.F. Doerge, J.B. Lippincott Company, Philadelphia, 1982.
2. Pharmaceutical Chemicals in Perspective, B.G. Reuben and H.A. Wittcoff, John Wiley & Sons, New York, 1989.
3. W.C. Foye, Principles of Medicinal Chemistry, Lea & Febiger, Philadelphia, U.S.A.
4. H. Singh and V. K. Kapoor, Medicinal and Pharmaceutical

CHL503-A
Self-Assembly Material

Credits: 3-0-0

SECTION-I

1. Non covalent interaction, Self-Assembled Supramolecular Polymers, Biological Self-Assembled Fibres and Layers, Amyloids, Actins and Fibrin, Bacterial S-Layers, Interfaces and Liquid Assemblies, Micelles and biological membrane, Metal–organic polyhedra and frameworks, Hydrogen bond assisted supramolecular assembly,Normal-phase chromatography,

SECTION-II

2. Self-Assembly in Synthetic Systems: Kinetic and Thermodynamic Considerations, Template Effects in Synthesis, Cooperativity and the Extended Site Binding Model, A Thermodynamic Model: Self-Assembly of Zinc Porphyrin Complexes, Cooperativity in oxygen transfer, Self-Assembling Coordination Compounds

3. Proteins and Foldamers: Single Molecule Self-Assembly, Strict Self-Assembly: The Tobacco Mosaic Virus and DNA

SECTION-III

4. Catenanes and Rotaxanes, Helical assembly, Supramolecular self-assembly for construction of Molecular motor, molecular switches, logic gate.

Reference

1. Supramolecular Chemistry. J. W. steed, J. L. Atwood, second edition 2009, Wiely.
2. Supramolecular Chemistry. Jean-Marie Lehn, 1995, Wiely.
3. Supramolecular chemistry-fundamental and applications. K. Ariga, T. Kunitake, 2006, Springer.

CHL504

Connection and Disconnection Approach in Organic Synthesis

Credits: 3-0-0

SECTION-I **16 Hours**

Disconnection approach:

An introduction to synthons and synthetic equivalents, disconnection approach, functional groupinterconversions

Strategies for disconnection approach

The importance of the order of events in organic synthesis, chemoselectivity, reversal of polarity, cyclisation reactions, protecting groups, stereoselectivity A and B, regioselectivity, use of acetylenes, carbonyl condensation and control in carbonyl condensation,

SECTION-II **16 hours**

Use of aliphatic nitro compounds, radical reaction, reconnections, Ring synthesis (3,4,5 and 6 membered), rearrangements, use of ketenes, pericyclic rearrangements

One group disconnections

One group C-X and C-C disconnections (alcohol and carbonyl compounds)

Two group disconnections

Two group C-X disconnections in 1,2-difunctionalized compounds,1,3-difunctionalized compounds and α,β-unsaturated carbonyl compounds, 1,4-difunctionalized compounds,

SECTION-III **13 Hrs**

1,5-difunctionalized compounds and 1,6-difunctionalized compounds

Synthesis using disconnection approach

Amine, alkene and aromatic heterocycles

Advanced strategy in disconnection approach

Choosing a disconnection, carbonyl disconnection, ring synthesis and advanced strategy

Books Suggested

1. Organic Synthesis: The Disconnection Approach by Stuart Warren, Paul Wyatt, Wiley; 2nd Edition edition.
2. Workbook for Organic Synthesis: Strategy and Control by Paul Wyatt, Stuart Warren, Wiley-Blackwell
3. Designing Organic Synthesis: S. Warren, Wiley.

4. Organic Synthesis-concept, methods and starting materials: J. Furhop and G. Penzillin, Verlage VCH.
5. Some Modern Methods of Organic Synthesis: W. Carruthers, Cambridge Univ. Press.
6. Modern Synthetic Reactions: H. O. House, W. A. Benjamin.
7. Principles Of Organic Synthesis: R.Norman and J. M. Coxon, Blackie Academic and professional.

CHL505
Chromatography and separation methods

Credits: 3-0-0

SECTION-I

1. Introduction to analytical separation, Principles of Adsorption Chromatography

2. Chromatographic Methods:

Classification of chromatographic methods according to separation and development procedure, Stationary phase, mobile phase, retention time.

SECTION-II

3. Gas chromatography:

Physical components, Types of column and detector, Carrier gas, Applications, Inverse Gas chromatography, GC-MS: construction and working.

SECTION-III

4. High performance liquid chromatography:

Construction and working, Partition chromatography, Normal and reverse phase chromatography, Ion exchange chromatography, Isocratic and gradient elution. Supercritical fluid chromatography: Mobile phase, Sample preparation, Drawback, Electrophoresis and electrochromatography

5. Gel permeation chromatography:

Working, Choice of Column: Organic column and aqueous column, Application, polydispersity index, Mark–Houwink equation.

6. Modern flash chromatography:

Advantage, comparison of column and flash chromatography

Reference

1. Chromatographic Methods, A. Braithwaite and F. J. Smith, 5th edn. Blackie Academic and rofessional, London, 1996.
2. Preparative chromatography, Henner Schmidt Traub, Wiely, 2005.
3. Principles of Instrumental Analysis, Skoog, Holler, Nieman, Fifth edition Thomson Books ,1998.

CHL506

Computer for Chemist

SECTION-I

I Introduction to Computers and Computing **8 Hrs**

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS. Data Processing, principles of programming. Algorithms and flow-charts.

SECTION-II

II Computer Programming in FORTRAN/C/BASIC **12 Hrs**

(The language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C and the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols. Expressions. Arithmatic assignment statement. Input and Output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBROUTINE. COMMON and DATA statements. (Students learn the programming logic and these language features by 'hands on' experience on a personal computer from the very beginning of this topic).

SECTION-III

Use of Computer Programmes **25 Hrs**

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Further, the students will operate one or two or the packages such as MATLAB, EASYPLOT, LOTUS, FOXPRO and Word Processing software such as WORDSTAR/MS-WORD.

CHP507
Biophysical Chemistry Lab

- Separation of a mixture of amino acids using thin layer chromatography
- Isolation and quantitation of DNA from onion
- Separation of proteins/DNA using size-exclusion chromatography (SEC)
- Separation of DNA using gel electrophoresis (agarose)
- Isolation, detection, and quantitation of protein (casein) from milk
- Separation of proteinsusingpolyacrylamide gel electrophoresis (SDS-PAGE)
- Osmosis and diffusion through semipermeable membrane
- Estimation of DNA quantity using UV-Vis spectrophotometer
- DNA/ligand interaction (Scatchard plot) using UV-Vis spectrophotometer
- Melting curves of DNA using UV-Vis spectrophotometer
- Serum albumin/ligand interaction using UV-Vis spectrophotometer
- Study of DNA conformation using circular dichroism spectroscopy
- Thermal stability and conformation of proteins using circular dichroism spectroscopy

Books recommended

- *Safety-Scale Laboratory Experiments for Chemistry for Today*, S L Seager and M R Slabaugh, Brooks/Cole Laboratory Series for General, Organic, and Biochemistry, VII edition, Brooks/Cole, 2010

CHP 508

Multi-step Organic Synthesis

The use of multi-step approach in organic synthesis and applications of spectroscopic techniques to determine the structures of the compounds prepared.

EXPERIMENTS

1. Synthesize (a) 2,4-dinitro-1-chlorobenzene from chlorobenzene, (b) mixture of *o*- and *p*-nitrophenols from phenol and (c) *p*-nitroacetanilide from acetanilide and make comparison of the reactivity of various substrates and reaction conditions used for performing nitration in each experiment. (Book 2, pp 978-979, 919-20)
2. Synthesis of 2-chloro-4-bromo-6-iodoaniline from aniline. (Book 1, pp 292-299)
3. Synthesis of benzalacetophenone by condensation of benzaldehyde with acetophenone and study its bromination and subsequent de-bromination. (Book 1, pp 242-247, Book 3 pp 361-365)
4. The epoxidation of benzalacetophenone to its epoxide and study its reactivity towards hydroxyl ion. (Book 3, pp 363-364).
5. Michael addition of aniline to benzalacetophenone. (Book 1, p 247)
6. Conversion of benzalacetophenone to its oxime and its transformation to amideand oxazole derivatives. (Book 1, pp 242-247, Book 3 pp 361-365)
7. Synthesis of anthranilic acid from phthalimide. (Book 2, pp 898-899)
8. Synthesis of *p*-aminobenzenesulfonamide. (Book 1, pp 275-289)
9. Synthesis of Methyl n-pentyl ketone from ethyl acetoacetate. (Book 2, pp 620-621)
10. Synthesis of triphenylcarbinol from bromobenzene. (Book 2, pp 540-541)

Books:

1. An Introduction to Modern Experimental Organic Chemistry, R.M. Roberts, Gilbert, L. B. Rodewaldand A.S. Wingrove. Holt, Ranehart and Winston Inc., J. C New York 1969.

2. Vogel's Text Book of Practical Organic Chemistry, 5th Edition.

3. Laboratory Experiments in Organic Chemistry, R. Adams, J.R. Johnson

CHL511

Advanced Organic Synthesis

Credits: 3-0-0

SECTION-I

Part-A Asymmetric synthesis **15 lectures**

Analytical methods for determination of enantiomeric purity – GC, HPLC and NMR. Natural sources of chiral starting materials, classification and methods of formation of new chiral compounds.

Part-B:- C-H activation using metal salts, Suzuki reaction, Heck reaction, Negishi coupling, Stille reaction, Sonogashira coupling reactions.

SECTION-II

Non-Enzymatic Approaches **15 lectures**

Methods of asymmetric synthesis using naturally occurring chiral compounds, nucleophile and electrophile bearing chiral auxillary, Diels – Alder cycloaddition and Claisen – cope rearrangements. Asymmetric carbon – carbon bond formation using alkylation, Michael reaction and addition to carbonyl compounds. Cram's rule and Felkin – Ahn model. Asymmetric oxidation and reductions.

SECTION-III

Organometallic synthesis in organic Catalysis **15 Lecture**

(a). Fundamental reaction steps of transition metal catalysed reaction. oxidative-addition reactions, elimination reactions, cleavage of C-H bonds, migration reaction, insertion reaction.

(b). Homo/heterogeneous catalysis by transition metal complexes.
Hydrogenation reaction, alkene isomerization, hydrosilylation and hydroboration reaction, alkene hydrogenation, reaction of CO and hydrogen, hydroformylation of unsaturated compounds, carbonylation reactions, C-C cross coupling and related reaction, reaction of conjugated dienes, reaction of alkynes, , alkene and alkyne metathesis, phase transfer catalysis,

Books

1. Some Modern Methods of Organic Synthesis by W Carruthers, Cambridge University Press.
2. Smith M B , March J March's Organic Chemistry 5th ed (2001)(2103s), Wiley, New York.

CHL512-B
Medicinal Chemistry-II

Credit 3-0-0

SECTION-I

Structure, stereochemistry, Mode of action, Structure activity relationships, specific clinical applications of following classes of pharmaceuticals with synthetic/commercial route to the indicated examples.

1. Antibacterials (13 Hrs)

Penicillines, Cephalosporins, Tetracyclines, Aminoglycosides, Chloramphenicol, Macrolides, Lincomycins, Polypeptides antibiotics, Polyene antibiotics. Sulfonamides and Sulfones fluoroquinolines, Trimethoprim and other unclassified antibiotics. Antimycobacterials: Sulfanilamides, p-Aminosalicyclic acid derivatives, Thioamides, Thiourea, derivatives, Thiosemicarbonazones, Isoniazid, Kanamycin sulfate, Capreomycin, Rifaampin, Pyrazinamide, Anthionamide, Clofazimine, Cyclosporin, Dapsone, Sulfazem.

Commercial synthetic / semi-synthetic routes to: 6-aminopenicillanic acid, ampicillin, amoxycillin, production of penicillin, 7-aminocephalsporanic acid, cephalexin, ceftizoxime, cefaclor, cephslothin, Tetracyclins: doxycycline, nalidixic acid, sulfadiazine, Norflaxacin, Ciproflexacin, O-flaxacin, Amiflaxacin, Difloxacin, Chloramphenicol, Nitroflurantion, Sulfamethyoxazole, Acetysulfoxiazole, Trimethoprim.

SECTION-II

2. Antiamoebic and Antiprotozoal Drugs (8 Hrs)

Emetine hydrochloride, 8-Hydroxyquinoline, Iodochlorohydroxyquinol, Metronidazole, Diloxanide furoate, Bilamical hydrochloride, Hydroxystilbamidine isothinate, Pentamidine isothionate, Nifurtimox,Suramin sodium, Carbarsone, Glycobiarsol, Melarsoprol, Sodium stibogluconate, Dimercaprool, Diethylcabamazine citrate, Centarsone, Acetarsone, Antimony potassium tartarate, Bismuth sodium thioglycollate, Sulphonamide, Stibiophen. Bismuth sodium thioglycollamate, Furazolidone.

Commercial synthetic routes to : Metronidozole, ronidazole, flunidazole, iodoquinol, nifurfimax, benzindazole, tryparsamide.

3. Antimalarials (7 Hrs)

Cinchona alkaloids, 4-Aminoquinolines, 8-Aminoquinolines, 9- Aminoacridines, Biguanides, Pyramidines and Sulfones, Mefloquine, Sulfonamides.

Commercial synthetic routes to : Chloroquine, pamaquine, primaquine, proguanil, Amodiaquine, Mefloquine, Pyremethamine, Sontoquine.

SECTION-III

4. Anthelmintics (8 Hrs)

Introduction, Tetrachloroethylene, Piperazines, Gentian violet, Pyrvinium pamoate, Thiabendazole, Mabendazole, baphenium hydroxynaphthoate, Dichlophene, Niclosamide, Levamisole hydrochloride, Tetramisole, Niridazole, Biothional, Antimonypotassium tartarate, Stibiophen, Sodium Stibiocaptate.

5. Antifungal Drugs (9 Hrs)

Fatty acids and their derivatives (Propionic acid, zinc propionate, sodium caprylate, zinc caprylate, undecylenic acid, Zinc undecylenate, Triacetin), Salicylanilids, Salicyclic acid, Tolnaftate, pchloromethoxylenol, Acrisocrin, Fluconazole, Itraconazole, Haloprogin, Clotrimazole, Econazole, Miconazole, Ketoconazole, Flucytosine, Griseofulvin, Polyene antibiotics (Nystatin, Amphoetericin-B), Chlorophenesin, Dithranol.

Commercial synthetic routes to: Miconazole, Clotrimazole, Econoazole, Fluconazole, Griseofulvin, Ketoconazole, Nafttidine, Tolnaftate, Flucytosin.

Books Recommended:

1. Wilson and Gisvolds Textbook of Organic Medicinal and Pharmaceuticals Chemistry, 8th edition, edited by R.F. Deorge, J.B. Lippincott Company, Philadelphia, 1982.

2. Pharmaceutical Chemicals in Perspective. B.G. Reuben and H.A.Wittcoff, John Wiley & Sons, New York, 1989.

3. W.O. Foye, T.L. Lamke, D.A. Williams, Principles of Medicinal Chemistry, 5^{th} Edition, Lippencott Williams and Wilkins, 2002.

CHL512A

Functional materials

SECTION-I

1. Advanced functional materials

Introduction to smart and functional materials: Challenges in the science and technology of advanced materials and its areas of applications.

2. Multifunctional hybrid materials

Introduction to hybrid materials, Discotic liquid crystalline dimers: structure – property relationships and applications, Supramolecular nanoassembly, supramolecular interactions, types of supramolecules, self-Assembled monolayers, Cationic, Anionic and Biomolecule receptors, and potential for supramolecular nanoassembly, Metal organic framework, structure, classification and its different applications.

SECTION-II

3. Carbon based hybrid composites

Introduction to composites, properties and its applications, composite materials based upon activated carbon, carbon aerogels, carbon nanotubes and 2D-graphene, Electrochemical performance of grapheme, Graphene composites, doping of grapheme with heteroatom, chitosan based materials and graphene.

4. Advanced biopolymers

Introduction to biopolymers, Synthetic biodegradable polymers, Quaternary polymers, polyethylenimine, Antimicrobial peptide mimics, Metal loading, synthesis of biopolymers by polycondensation, General polycondensation techniques, Post polycondensation techniques, chain extension technique and enzyme catalysed condensation and its applications.

Section-III

5. Advanced energy materials

Introduction to new generation of materials for sustainable energy, fundamentals of organo metal halide perovskite cells, deposition methods and crystal engineering, Dye (Quantum) sensitized solar cells, bulk heterojunction solar cells, supercapacitors, introduction to hydrogen storage materials.

Recommended readings:

1. *Advanced functional materials* (Scrivener publishing, *Wiley interscience*), Ashutosh Tiwari, Lokman Uzun, **2015**.

2. *Advanced functional materials* (Zhejiang university press, *Springer*), Hee-Gweon Woo, Hong Li, **2011**.

3. *Functional Materials: Preparation, Processing and Applications* (*Elsevier*), S. Banerjee and A.K. Tyagi, **2012**.

4. *Advanced functional materials*, Volume 2, 1st edition (*Elsevier*), Biplab Sanyal and Olle Eriksson, **2012**.