

Dr. B. R. AMBEDKAR NATIONAL INSTITUTE OF TECHNOLOGY JALANDHAR

DEPARTMENT OF CHEMISTRY

SCHEME AND SCHEDULE OF COURSES
M Sc IN CHEMISTRY
SEMESTER I

| Course Code | Course Title | Hours /week | | | Credits |
|---------------------------|--|-------------|---|---|---------|
| | | L | T | P | |
| CY-512 | Stereochemistry and Reaction Mechanism | 3 | 1 | 0 | 4 |
| CY-521 | Thermodynamics and Chemical Kinetics | 3 | 1 | 0 | 4 |
| CY-532 | Main Group Chemistry | 3 | 1 | 0 | 4 |
| CY-541 | Intellectual Property Rights | 2 | 0 | 0 | 2 |
| CY-542 | Basic Biological Chemistry / | 2 | 0 | 0 | 2 |
| MA-551 | Mathematics for Chemists | | | | |
| CY-561 | Organic Chemistry Lab | 0 | 0 | 8 | 4 |
| CY-571 | Computational Skills , Graphics & Simulation Lab | 0 | 0 | 4 | 2 |
| CY-599 | Seminar I | 0 | 0 | 0 | 0 |
| Total = 22 Credits | | | | | |

SEMESTER II

| Course Code | Course Title | Hours /week | | | Credits |
|---------------------------|---|-------------|---|---|---------|
| | | L | T | P | |
| CY-511 | Quantum Chemistry | 3 | 1 | 0 | 4 |
| CY-513 | Pharmaceutical Chemistry | 2 | 0 | 0 | 2 |
| CY-522 | Surface Chemistry, Adsorption and Catalysis | 3 | 1 | 0 | 4 |
| CY-531 | Principles of Organic Synthesis | 3 | 1 | 0 | 4 |
| CY-551 | Symmetry and Group Theory | 2 | 0 | 0 | 2 |
| CY-562 | Physical Chemistry Lab | 0 | 0 | 8 | 4 |
| CY-592 | Electronics for Chemists Lab | 0 | 0 | 4 | 2 |
| Total = 22 Credits | | | | | |

CY-597 Summer Training in Research Lab/Industry (after second semester) 0 0 4 2

Note : Earlier known as Practical Training in Research Lab/Industry (CY- 597)

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DEPARTMENT OF CHEMISTRY

SCHEME AND SCHEDULE OF COURSES
M Sc IN CHEMISTRY
SEMESTER III

| Course Code | Course Title | Hours /week | | | Credits |
|---------------------------|--|-------------|---|---|---------|
| | | L | T | P | |
| CY-582 | Inorganic Chemistry Lab | 0 | 0 | 8 | 4 |
| CY-600 | Project Phase -I | 0 | 0 | 4 | 2 |
| CY-611 | Chemistry of Transition and Inner- transition Elements | 3 | 1 | 0 | 4 |
| CY-621 | Physical Methods of Structure Elucidation | 3 | 1 | 0 | 4 |
| CY-631 | Analytical Principles and Instrumental Methods of Analysis | 3 | 1 | 0 | 4 |
| CY-6XX | * Elective- I | 3 | 1 | 0 | 4 |
| Total = 22 Credits | | | | | |

SEMESTER IV

| Course Code | Course Title | Hours /week | | | Credits |
|---------------------------|--|-------------|---|----|---------|
| | | L | T | P | |
| CY-596 | Comprehensive Viva | 1 | 0 | 0 | 1 |
| CY- 598 | Scientific Documentation and Presentation Skills | 0 | 0 | 2 | 1 |
| CY-599 | Seminar II | 1 | 0 | 0 | 1 |
| CY-600 | Project Phase - II | 0 | 0 | 16 | 8 |
| CY – | **Elective-II | 3 | 1 | 0 | 4 |
| CY – | **Elective -III | 3 | 1 | 0 | 4 |
| CY-6XX | * Elective –IV | 3 | 0 | 0 | 3 |
| Total = 22 Credits | | | | | |

TOTAL CREDITS= 22+22+22+22=90

*The Open Elective i.e. Research Methodology (ID-601) has been replaced with Electives : Polymer Chemistry (CY-623) and Drug Design and Development (CY-671) duly approved by Chairman Senate and will be of 03 credits.

** Electives may be chosen by the student out of the electives offered by the Department/ Institute depending on the availability of faculty.

Dr. B. R. AMBEDKAR NATIONAL INSTITUTE OF TECHNOLOGY JALANDHAR

DEPARTMENT OF CHEMISTRY

LIST OF COURSES FOR M. Sc. / Ph D CHEMISTRY STUDENTS

| Course Code | Course Title | Hours /week | | | Credits |
|-------------|---|-------------|---|---|---------|
| | | L | T | P | |
| CY-612 | Natural Products | 3 | 1 | 0 | 4 |
| CY-622 | Ligand Field Theory | 3 | 1 | 0 | 4 |
| CY-623 | Polymer Chemistry | 3 | 1 | 0 | 4 |
| CY-632 | Bioinorganic Chemistry | 3 | 1 | 0 | 4 |
| CY-633 | Advanced Inorganic Chemistry – I | 3 | 1 | 0 | 4 |
| CY-634 | Advanced Inorganic Chemistry – II | 3 | 1 | 0 | 4 |
| CY-641 | Solid State Chemistry | 3 | 1 | 0 | 4 |
| CY-650 | Nanochemistry | 3 | 1 | 0 | 4 |
| CY-651 | Photochemistry | 3 | 1 | 0 | 4 |
| CY-652 | Environmental Chemistry | 3 | 1 | 0 | 4 |
| CY-653 | Statistical Thermodynamics | 3 | 1 | 0 | 4 |
| CY-661 | Nanomaterials, Nanoscience & Nanotechnology | 3 | 1 | 0 | 4 |
| CY-662 | Industrial Organic Chemistry | 3 | 1 | 0 | 4 |
| CY-665 | Leather Chemicals | 3 | 1 | 0 | 4 |
| CY-671 | Drug Design and Development | 3 | 1 | 0 | 4 |
| CY-681 | Mechanistic Inorganic Chemistry | 3 | 1 | 0 | 4 |

LIST OF COURSES EXCLUSIVELY FOR Ph D CHEMISTRY STUDENTS

| Course Code | Course Title | Hours /week | | | Credits |
|-------------|--|-------------|---|---|---------|
| | | L | T | P | |
| CY-761 | Principles of Instrumental Methods of Analysis | 3 | 1 | 0 | 4 |
| CY-771 | Advanced Spectroscopy | 3 | 1 | 0 | 4 |
| CY-781 | Chemistry of Materials | 3 | 1 | 0 | 4 |
| CY-791 | Macromolecular Chemistry | 3 | 1 | 0 | 4 |

LIST OF OPEN ELECTIVE COURSES FOR B. TECH STUDENTS

| Course Code | Course Title | Hours /week | | | Credits |
|-------------|---|-------------|---|---|---------|
| | | L | T | P | |
| CY-583 | Molecule as Electronics Devices | 3 | 1 | 0 | 4 |
| CY-623 | Polymer Chemistry | 3 | 1 | 0 | 4 |
| CY-661 | Nanomaterials, Nanoscience & Nanotechnology | 3 | 1 | 0 | 4 |

SEMESTER - I

L T P C
3 1 0 4

CY-512 Stereochemistry and Reaction Mechanism

- 1. Stereochemistry:** Configuration and chirality, optical isomerism, R,S-convention, enantiotopic and diastereotopic groups, methods of resolution,. Geometrical isomerism E,Z-convention. Conformational & configuration of cyclic compounds, Atropisomerism, Atropisomerism about $sp^2 - sp^2$ bond, $sp^3 - sp^3$ bond, $sp^2 - sp^3$ bond, Molecular propeller & Gears.
- 2. Reactive Intermediates:** Generation, structure and reactions of carbocations, carbanions, nitrenes and free radicals.
- 3. Nucleophilic substitution:** Mechanisms, Classical and nonclassical carbocations. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium. Aromatic Nucleophilic substitution: Mechanisms, reactivity, effect of substrate structure, leaving group and attacking nucleophile.
- 4. Electrophilic Substitution:** Mechanisms, effect of substrates, leaving group and the solvent polarity on the reactivity. Aromatic- the Arenium ion mechanism, orientation and reactivity, energy profile diagrams, quantitative treatment of reactivity in substrates and electrophiles.
- 5. Addition to Carbon-Carbon Multiple Bonds:** Mechanism, direction and stereochemistry, addition to alkenes and alkynes, Transition metal organometallics.
- 6. Addition to Carbon-hetero Multiple Bonds;** Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles, Addition of Grignard reagents.
- 7. Elimination Reactions:** Reaction mechanism, Direction, stereochemistry, formation of alkenes , alkynes and other multiple bonds.
- 8. Ring Expansion and Contraction:** Demjanov ring expansion, Favorskii rearrangement.

REFERENCES:

1. Stereochemistry of Carbon Compounds, E. J. Eliel, Tata Mc Graw Hill, Ed. 2002.
2. Stereochemistry of Organic Compounds, D. Nasipuri, Wiley, Ed. 1994
3. Organic Chemistry, J. M. Hornback, Books Coley, Ed. 1998.
4. Organic Chemistry, P. Y. Bruice, Prentice Hall, Ed. 1998.
5. Organic Reaction and Their Mechanisms, P. S. Kalsi, New Age International Publishers, 2nd Ed. 2007.
6. Modern Synthetic Reactions, H. O. House and W. A. Benjamin, Inc, Ed. 1972.

CY-521 Thermodynamics and Chemical Kinetics

- 1. Law of Thermodynamics:** Exact and Inexact Differentials, Cyclic Rule, Reciprocity Characteristics, Homogenous Function, Euler's Theorem, third Law of thermodynamics, Nernst Heat theorem, Thermodynamic Properties at Absolute Zero, Entropy & Third Law of Thermodynamics.
- 2. System of Variable Compositions:** Partial Molar Quantities, Chemical Potential and its Variation with Temperature and Pressure, Chemical Potential of Real Gases & Fugacity, Chemical Potential in ideal Gas Mixture, Concept of Escaping Tendency.
- 3. Physical Transformation of Pure Substances and Simple Mixtures:** Phase Diagrams, Phase Stability and Phase Transitions, The Physical Liquid Surface, Thermodynamics function of Mixing.
- 4. Chemical Equilibrium:** Spontaneous Chemical Reactions, Response of Equilibria to the Conditions, Thermodynamic Properties of Ions in Solution.
- 5. Chemical Kinetics:** Collision theory of Reaction Rates, Arrhenius Equation and Activated Complex Theory, Comparison of Collision and Activated Complex Theory.
- 6. Advanced Chemical Kinetics:** Applications of Activated Complex Theory, RRK and RRKM Theory, Theories of Unimolecular Reactions.
- 7. Dynamics of Complex Reactions:** Ion-Ion Reactions, Ion-Dipole reactions, Enzyme Kinetics, polymerization Kinetics, Kinetic Salt, Salt Effect.
- 8. Dynamics of Fast Reactions:** General Treatment of Chain Reactions, Theories of Branching Chain and Explosion, Flow Methods, Relaxation Techniques, Flash Photolysis.

REFERENCES:

1. *Thermodynamics A core Course* by R. C. Srivastva, S. K. Saha, A. K. Jain, PH I, New Delhi, **2007**.
2. *Physical Chemistry*, P. Atkins, J. D. Paula, Oxford University Press, 7th Indian Edition, **2007**.
3. *An Introduction to Chemical Thermodynamics* by R. P. Rastogi & R. R. Mishra, Vikas Publishing House, 6th Edition, **2007**.
4. *Chemical Kinetics* by Keith J. Laidler, Pearson Education, 3rd Edition.
5. *Chemical Kinetics* by K. A. Corrnors, VCH, **1998**.
6. *Physical Chemistry* by R. S. Berry, S. A. Rice & J. Ross, Oxford University Press 2nd Edition, **2000**.
7. *Fast Reactions* J. N. Bradley, Oxford University press, **1975**.

Prepared By: Dr. Harsh Kumar

Ratified By: Dr. Rajeev Jindal

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CY- 532

Main Group Chemistry

- 1. Chemistry of hydrogen:** Ionized forms of Hydrogen, Protonic acids and bases, The Hydrogen Bond, its influence on Properties and influence on structure, Strength of hydrogen bonds and theoretical description.
- 2. Chemistry of S-block metals:** Hydrides, Halides, Oxides, Peroxides, Superoxides, Suboxides, Hydroxides, Oxoacid salts Complexes Crowns and Crypts of Alkali Metals and coordination complexes of Alkaline Earth Metals.
- 3. Chemistry of Boron and Aluminum:** Boranes, Bonding in boranes, topology of boranes, synthesis and reactivity. Carboranes and mettallocarboranes, Borazine and boron nitride. Chemistry of Aluminum Halides. Aluminum Alkyls. Low oxidation state Al compounds.
- 4. Chemistry of Silicon:** Organosilicon Compounds. Silicates and Aluminosilicates. Low-valent Silicon compounds, silylenes and R_3Si^+ .
- 5. Inorganic rings, Cages, Clusters and Polymers:** Phosphazenes, Cyclophosphazenes, Polyphosphazenes and the polymers derived from them. Polysilanes.
- 6. Chemistry of halogens and noble gases:** Inter Halogens, Poly Halide Anions, CFC's, Ozone layer and Clathrates.
- 7. Chemistry of group 12 elements:** Halides & Oxygen compounds, chalcogenides & Related compounds, low-valent compounds & Formation of coordination complexes.

References:

1. *Main Group Chemistry*, W. Henderson, Royal Society of Chemistry, **2000**.
2. *Advanced Inorganic Chemistry*, F. A. Cotton and G. Wilkinson et. al, Sixth edition John Wiley & Sons, **2003**.
3. *Inorganic Chemistry*, J. E. Huheey et. al, Fourth edition, Pearson, **2005**.
4. *Concepts & Model of Inorganic Chemistry*, B. Douglas et. al, 3rd John Wiley & Sons, **2001**.
5. *Chemistry of Elements*, N. N. Greenwood, Pergamon Press, **2000**.
6. *Inorganic Chemistry 4th edition* D. F. Shriver and P. W. Atkins, Oxford University, Oxford, **2006**.

L T P C
2 0 0 2

CY-541 Intellectual Properties Rights

1. **Introduction:** Intellectual property rights, promotion and protection concepts, classification, copyright and trade marks.
2. **W T O and W I P O:** Structure, functions and mandate.
3. **Patents:** Difference between discovery and invention Patentable inventions, right of patent owner.
4. **Copy Right and Trade Mark:** Difference, advantages and limitations.
5. **Geographical Indicators:** Geographical indicators and their protection, difference between geographical indication and trademark.
6. **Industrial Design:** Industrial design, protection of industrial design.
7. **Traditional knowledge:** Scope and limitations.
8. **TRIPS Agreement:** Salient features, duration and transitory provisions.
9. **National and International Registration Systems:** The patent corporation treaty (the PCT), main international agreements.
10. **Indian Patent Rules:** The Patents Act 1970, The Patent Rule 2003 as amended and effective from 1.1.2005, salient features.

REFERENCES:

1. *Copyright Law*, Vaver, Dav, Toronto: Irwin Law, , ISBN 1-55221-034-0, **2000**.
2. *Intellectual Property*, Drahos , Peter, Adlershot et.al. Darmouth, , ISBN 1840147407, **1999**.
3. *Intellectual Property: Patents, Copyright trade marks and allied rights*, Cornish, William R , London: Sweet and Maxwell, 4th dition , ISBN: 0421635401,**1999**.
4. *Intellectual Property Reading Material*, World Intellectual Property Organization, 2nd edition, ISBN: 92-805-0756-7,**1998**.
5. *Patents, trademarks, and related rights; national and international protection*, Ladas, Stephen P, Cambridge, MA: Harvard University Press, ISBN: 06746577756, **1975**.
6. *Universal's The Patent Act (39 of 1970) with amendments*-Universal Law publishing **2005**.

Website of WTO and WIPO for current & updated materials

DL 001 and DL-101 courses of WIPO

Prepared By: Dr. S B S Mishra
Ratified By: Dr. B S Kaith

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CY-542

Basic Biological Chemistry

- 1. Cell:** Types of cells, structure and functions
- 2. Introduction to Biomolecules:** Carbohydrates, Proteins, Amino acids, Lipids and phospholipids.
- 3. Nucleic Acids:** Base pairing, double helices, DNA replications, transcription and translation.
- 4. Enzymes:** Enzyme kinetics and mechanism, nature and application of enzymes.
- 5. Health, Diet and Environment:** Nutritional requirements (recommended dietary allowances, major nutrients: sources of energy, carbohydrates, fats, proteins, vitamins, mineral and trace elements), cholesterol: friends or foe, diet and weight, nutrition and cancer, interaction between food and drugs, Biological membranes and transport mechanism, waste water and sewage treatment, landfill technologies.

REFERENCES:

1. Lehninger Principles of Biochemistry, David L. Nelson and Michal M. Cox, CBS Publisher, Ed. 2009.
2. Biotechnology, J. E. Smith, Cambridge University Press, 5th Ed. 2009.
3. Principles of Biotechnology and Genetic Engineering, A. J. Nair, University Science Press, New Delhi, 2nd Ed. 2010.
4. Principles of Biochemistry, T. N. Pattabiraman, Gajanana Book Publishers and Distributors, 3rd Ed. 2001.
5. Elements of Chemistry, General, Organic and Biological, Robert S. Boikess, Kenneth Breslauer and Edward Edelson, Prentice-Hall, New Jersey, Ed. 1986.

Prepared By: Dr B S Kaith

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MA-551

Mathematics for Chemists

1. **Matrices:** Matrix addition, subtraction and multiplication, transpose of a matrix, inverse of a matrix, solution of simple linear equations by matrices.
2. **Vectors:** Scalar and vector quantities, vector addition and law of addition, commutative and associated law, vector multiplication. Vector differential operator Del, Gradient, Divergence and Curl.
3. **Functions:** Real functions, operations on Real functions, Intervals (closed and open) Even and odd functions, periodic function.
4. **Limits:** Introduction, Units, Formal Approach to limit, Algebra of limits, Evaluation of limits.
5. **Continuity:** Continuous function, Continuity in an interval, Properties of continuous function. Domain of continuity.
6. **Differential Calculus:** Differentiation from 1st principle of x^n , $(ax + b)^n$, $\log x$, $\sin x$, $\cos x$, $\tan x$. Rules of differentiation and application to simple function of the form $y = f(x)$, Implicit differentiation and parametric differentiation, Differentiation by using trigonometric function. Differentiation of a function with respect to another function. Partial differentiation, Euler's theorem, concept of Maxima and Minima for simple function of the type $y = f(x)$.
7. **Integral Calculus:** Integration of some standard functions including trigonometric function, Integration by parts, substitution and partial fractions.
8. **Differential Equation:** Definition and formation of differential equations, solution of differential equations of first order and first degree: variable separable, homogeneous function Leibnitz's linear equations.

REFERENCES:

1. *Advanced Engineering Mathematics*, Erwin Kreyszig, 8th edition, John Wiley & Sons Inc.
2. *Advanced Engineering Mathematics*, R. K. Jain, S. R. K. Lyengar, Narosa Publishing House.
3. *Advanced Engineering Mathematics*, D. G. Zill, M. R. Cullen, 2nd Edition, CBS Publishing & distributions.

Prepared By: Dr. Geeta Partap
Ratified By: Dr. Jaspal Singh

CY- 561

Organic Chemistry Lab

1. Distillation & separation

- (a) To purify common organic solvents
- (b) Extract rose oil from rose petals by steam distillation.
- (c) Separation of given mixtures.

2. Chromatography

- (a) To separate plant pigments by column chromatography.
- (b) Identification of phytoconstituents using thin layer chromatography.
- (c) Identification of sugars in fruit juices through paper chromatography.

3. Organic analysis:

Detection of common functional groups in the given organic compounds and identification of compound through derivatives.

4. Organic preparations:

- 1. Cinnamic acid by perkin reaction
- 2. Benzaldehyde by Beckmann rearrangement
- 3. Chalcone by Aldol condensation
- 4. Ethyl p-aminobenzoate (benzocaine)
- 5. Preparation of Benzopinacolone by Pinacol-Pinacolone rearrangement
- 6. Synthesis of N-phenylmaleimide
- 7. Preparation of p-bromoaniline from acetanilide.
- 8. Preparation of Phenacetin from p-aminophenol
- 9. Preparation of eosin from phthalic anhydride
- 10. Preparation of p-chlorobenzoic acid from p-toluidine.

5. Biochemical preparations/ Estimations

- 1. Determination of acid value of oils.
- 2. Determination of Saponification value of given oil/ fat.
- 3. Determination of Iodine number of fat.
- 4. Isolation of casein from milk.
- 5. Isolation of Caffeine from tea Leaves.

6. Quantitative analysis

- 1. Estimation of glucose in the given sample.
- 2. Estimation of number of amino groups in aniline.

7. Physical method Determination

The synthesized compounds will be characterized on the basis of ^1H , ^{13}C , U.V, I.R, Mass & CHNS analyser.

REFERNCES:

1. *An introduction to Practical Biochemistry*-David T. Plummer , third Edition, Tata McGraw Hills, **1998** .
2. *Text Book of Practical Organic Chemistry* – A. I. Vogel, Pearson education, 5th Edition, **2005**.
3. *Experimental Organic Chemistry*, Vol 2, P. R. Singh ,D .S. Gupta and K.S. Bajpai, Tata Mc Graw Hill, **1981**.
4. *Practical Organic Chemistry* – G Mann, B. C. Saunders, ELBS Edition, **1989**.
5. *Advanced Practical Organic Chemisry*, N. K. Vishnoi, Vikas publishing House Pvt. Ltd. , 2nd edition, **1994**.

Prepared By: Dr. Jaspreet Rajput
Dr. B S Kaith
Dr. N C Kothiyal

CY-571 Computational Skills, Graphics & Simulation Lab

1. **MS Office:** MS Word, MS Excel, MS Power Point, Basic features of Power Point; Presentation.
2. **Chemwind / Chemdraw:** Drawing and editing molecular structures using Chemwind and Chemdraw templates.
3. **Programming in C Language:** Introduction, writing programmes in C language, Exercises in C language. Features of C++ and Visual C.
4. **Introduction to Web and Internet:** LAN and E-mail, Importance of Internet; Types fo search engines: Basic components of browsing page; importance of networks; networking personal computers; importance of E-mailing, search engines in chemical sciences.
5. **Computer Graphics:** Computer-aided design, Presentation graphics, Computer art, Entertainment, Education and training, Visualization, Image processing, Graphical user interfaces.
6. **Numerical Methods and Simulation:** Numerical methods in chemistry, Mathematical modeling of reactions and their simulation, Analysis and synthesis of chemical systems.
7. **Computer Animation:** Design of animation sequences, General computer animation, Kinematics and Dynamics.

REFERENCES:

1. *MS Office made easy*, supplied by Microsoft Inc.
2. *Information Technology-The breaking wave*, Curtin, Fuley Sen and Morin, TMH 1999.
3. *Donald Hearn and M Pauline Baker "Computer Graphics" 2nd edition*, Prentice Hall, 1996.
4. *JCE Software*, Journal of Chemical Education, American Chemical Society.

L T P C

**CY-599 Seminar I
(Compulsory for M. Sc. 1st year)**

SEMESTER - II

CY-511**Quantum Chemistry**

1. **Foundations of Quantum Mechanics:** Operators, Postulates, Matrices and Schrodinger Equation.
2. **Linear Motion and harmonic Oscillators:** Translational, harmonic, particle in a box a penetration through barriers.
3. **Rotational motion and hydrogen atom:** Particle in a ring & on a sphere, motion in a columbic field.
4. **Angular momentum:** Angular momentum operators, definition of states, Composite systems.
5. **Techniques of Approximation:** Perturbation theory, variation theory, HF theoretic, time dependent perturbation.
6. **Atomic Structure:** Hydrogen, Helium & multi electron system.
7. **Molecular Structure:** Born- openheimer approximation MO theory of mono, dia & polyatomic molecules, band theory of solids.
8. **Electronic Structure:** SCF method electron correlation Density functional theory, gradient method, semi-empirical methods & software packages for calculations.
9. **Molecular Rotation & Vibration:** Rotation & Vibration in diatomic, polyatomic molecules.
10. **Electronic Transition in molecules:** Rotational, Vibronic and electronic states & fates of excited species.

REFERENCES:

1. *Quantum Chemistry*, I. N. Levine, Prentice Hall, **2000**.
2. *Molecular Quantum Mechanics*, P. W. Atkins and R. S. Friendman, OUP, **1997**.
3. *Physical Chemistry*-by P. W. Atkins, Oxford University Press, **1990**.
4. *Introduction to Quantum Mechanics with Applications to Chemistry*, L. Pauling and E. B. Wilson, Dover NY, **1985**.

Prepared By: **Dr. S B S Mishra**
Ratified By: **Dr. Harsh Kumar**

L T P C
2 0 0 2

CY –513 Pharmaceutical Chemistry

1. **Drug Discovery and Drug Development:** Introduction, Present and Past, Drugs and the medicinal chemist, Classification of drugs, Drug targets specification, Choice of Bioassay, In Vivo and in Vitro tests, Pit falls.
2. **Drug Action at Receptors:** Receptor role, Neuro-transmitters and Hormones, Change of shape by the receptors, Design of Agonists and Antagonists, Drug action on DNA and RNA.
3. **Drug Design, Drug-Target Interactions:** Introduction, Variation of Substituent, Expansion of the Structure, Chain expansion/Contractions, Ring expansion/Contractions, Ring Variation, Ring Fusions, Isosteres.
4. **Pharmacokinetics:** Drug distribution and survival, Pharmacokinetic issues in drug design like Chemical and Metabolic stability, Hydrophilic / hydrophobic balance, Ionization, size and number of hydrogen bonding interactions, Drug dose levels, solubility and membrane permeability, variation of different groups to alter polarity.
5. **Prodrugs:** Introduction, Effect of prodrugs on: improved membrane permeability, prolonged drug activity, masking drug toxicity and side effects, increased chemical stability, targeting of drugs, prodrugs activation by external influence.
6. **Drug administration:** Introduction, oral administration, sublingual administration, rectal administration, epithelial administration, inhalation, injection and implants.

REFERENCES:

1. *Textbook of Pharmacology*, W. C. Bowman, and M. J. Rand, Blackwell Scientific **1980**.
2. *Medicinal Chemistry-the role of organic chemistry in drug*, C. R. Ganellin, and S. M. Roberts, , *research*, Academic Press **1993**.
3. *Medicinal Chemistry-principles and practice*, F. D. King, , The Royal Society of Chemistry **1994**.
4. *Burger's Medicinal Chemistry and drug discovery*, M. E. Wolff, *5th edition* Volume 1-5. Wiley **1995**.

Prepared By: Dr. B S Kaith
Ratified By: Dr. Jaspreet Rajput

CY-522 Surface Chemistry Adsorption and Catalysis

1. **Introduction:-**Basics of surface chemistry, surface tension and adsorption
2. **Surface & Colloids:** Coagulation and kinetics of coagulation, spontaneous aging of colloids.
3. **Aggregation Processes:** Coalescence and particle growth, Stability of colloids, Electric properties, theories of structure of electrical double layer, determination of change on colloids particle, size and shape of colloids particles.
4. **Association of colloids:** Self - assembly system, Reversal of phase, emulsion, Macro and Micro emulsion and Aerosols, emulsifying agents, theories of emulsification, gels, sol gel transformation thixotropy.
5. **Electrokinetic Effect:** Electrosmosis, electrophoresis, streaming potential, Dorn effect, stabilization of surfactant solutions.
6. **Adsorption:** Adsorption of gases by solids, solids from solution ,measurement of adsorption factors affecting adsorption, Adsorption Isotherms, , Gibbs adsorption equation, surface films.
7. **Catalysis:** Homogenous and Heterogeneous Catalysts, Acid base catalysis, Biocatalysts, Micellar catalysis, Mechanism of few catalytic reactions.
8. **Nanoscience :**Creation ,Evaluation and Application

REFERENCES:

1. *Basic Principles of Colloids Science*, D. H. Everthi, Royal Society of Chemistry, **1988**.
2. *Basic Physical Chemistry*, W. J. Moore, Printice Hall of India, **1986**.
3. *Surface*, G. Attard and C. Barners, Oxford Science Publications, **1998**.
4. *Physical Chemistry*, 3rd edition , G. W Castellan, Narosa, **2002**.
5. *Basic and Application of Heterogeneous Catalysis*, by M. Booker, Oxford Science Publication, **1998**.
6. *Physical Chemistry of Surfaces*, A. W. Adamoson.

CY-531 Principle of Organic Synthesis

- 1. Energetic, Kinetics, and the Investigation of Mechanism:** Energetic, rate and activation energy of reaction, kinetics and the rate limiting step, kinetic and thermodynamic control, investigation methods.
- 2. Phase Transfer Catalysts:** Introduction, mechanism, types and advantages, preparation of catalysts & application.
- 3. Crown Ethers:** Introduction, nomenclature, special Features, nature of donor site and synthetic applications.
- 4. Reagents in Organic Synthesis:** Anhydrous aluminium chloride, aluminium isopropoxide, boron trifluoride, N-Bromosuccinimide Diazomethane, Fenton's Reagent, Hydrogen peroxide, Lead tetra acetate, Lithium Aluminium Hydride, Osmium Tetroxide, Perbenzoic acid (Peroxybenzoic acid), periodic acid, Raney nickel, selenium dioxide, sodium amide (sodamide), sodium borohydride, NaBH₄, Wilkinson's catalyst.
- 5. Name Reactions:** Aldol condensation, Allylic Rearrangement, Baeyer- Villiger Rearrangement, Beckmann Rearrangement , Birch Reduction, Cannizzaro Reaction, Claisen condensation and rearrangement, Curtius reaction, Diels Elders Reactions, Fries Rearrangement, Hofmann Rearrangement, Mannich Reaction, Oppenauer Oxidation, Pinacol-Pinacolone Rearrangement, Reformatsky Reaction, Reamer Tieman Reaction.
- 6. Pericyclic Reaction:** Introduction, electrocyclic reactions, theoretical explanation, conservation of orbital symmetry, cycloadditon reactions, frontier molecular orbital approach, sigmatropic rearrangements.
- 7. Ring closure and opening reactions:** Formation and opening of rings, Diekmann reaction, Baldwin Rules, Robinson-Annellation, Michael-Robinson addition Thorpe Ziegler reaction, Acylation Cycloaddition, Diels-Alder reaction, Simmons-Smith reaction

REFERENCES:

1. Organic Synthesis - The Disconnection Approach, S. Warren, Willey Interscience, Ed. 1982.
2. Reactions Rearrangements and Reagents, S. N. Sanyal, Publisher Bharti Bhawan, 4th Ed. 2008.
3. Organic Synthesis-special Techniques, V. K. Ahluwalia and R. Aggarwal, Narosa Publishing House, Ed. 2005.
4. A Guidebook to Mechanism in Organic Chemistry, P. Sykes, 6th Ed. 1981.
5. Practical Organic Chemistry, B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, Pearson, 5th Ed. 2002.
6. Phase Transfer Catalysis: Principles and Techniques, C. M. Starkes and C. Liotta, Acedemic Press, Ed. 1998.
7. Crown Compounds Their Characteristics and Applications, M. Iraoka, Amesterdam, Ed. 1982.

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CY-551 Symmetry and Group Theory

1. **Symmetry elements and operations** : Symmetry planes and Reflections, Inversion centre, Proper axes and Proper rotations, Improper axes and Improper rotations.
2. **Relations among Symmetry elements** : Products of symmetry operations, Equivalent symmetry elements and Equivalent atoms, General relations among symmetry elements and operations, symmetry point groups, symmetry classification of molecules.
3. **Representations of groups** : Important rules about irreducible representations and their characters, Relationship between reducible and irreducible representations with examples, construction of character tables.
4. **Molecular orbital theory and its applications** : Symmetry based selection rules for cyclisation reactions, Dimerization of ethylene, Diels-Alder reactions.
5. **Molecular orbital theory for inorganic compounds** : Transformation properties of atomic orbitals, Molecular orbitals for sigma bonding in tetrahedral and octahedral molecules.
6. **Ligand Field theory** : Introduction, Electronic structure of free atoms and ions, splitting of levels and terms in a chemical environment, construction of energy level diagram.

REFERENCES:

1. *Chemical Applications of Group Theory*, F. A. Cotton, Wiley, 3rd edition, **2004**.
2. *Valence Theory*, J.N. Murrell et. al, John Wiley **1970**.
3. *Conservation of Orbital Symmetry*, R. B. Woodward and R. Hoffmann Academic Press **1970**.
4. *Introduction to Ligand Fields*, B .N. Figgis, John Wiley **1996**.

Prepared By: Dr. S B S Mishra
Ratified By: Dr. Sangeeta Obrai

CY-562 Physical Chemistry Lab

1. Properties of liquids and solutions.

- (a) To find the molecular weight of a non-volatile solute (urea) by Beckmann freezing point depression method
- (b) To determine the degree of ionization of sodium chloride at different concentration of its aqueous solution by the depression of freezing point.
- (c) To find refractive index and molecular refractivity of organic liquids.
- (d) To determine the densities and speeds of sound of binary and ternary liquid mixtures with the help of densimeter.
- (e) To determine the viscosities of binary and ternary liquid mixtures with the help of viscometer.

2. Chemical Kinetics

- (a) To determine specific rate of acid catalyzed hydrolysis of Ethyl, Acetate at 248.15°K.
- (b) To determine the specific rate of the hydrolysis of Ethyl acetate by Sodium Hydroxide at 298.15°K.
- (c) To study the rate of acid catalyzed iodination of acetone in the presence of excess acid and action at 298.15°K.

3 Surface chemistry and colloids

- (a) To determine the surface tension and parachor of benzene / toluene
- (b) To find out interfacial tension (IFT) between tow immiscible liquid using Dunoy's / auto Tensiometer and effect of salt concentration on IFT.
- (c) To study adsorptions isotherms of acetic acid from their aqueous solution by charcoal.
- (d) To study the variation of surface Tension of Eezee detergent with concentration and to find its CMC.
- (e) To find out coagulant doses with the help of flocculator for different samples.
- (f) To remove colloidal particles from potable water.

4. Thermodynamics

- (a) To determine heat of neutralization of hydrochloric acid and sodium hydroxide
- (b) To determine the solubility product of Barium iodate.

5. Thermo Analytical Methods

- (a) To study thermal decomposition of copper sulfate pentahydrate
- (b) To study the precipitation reaction between silver nitrate and sodium chloride.

6. Spectrophotometry

- (a) To verify Beer's law for solution of KMnO_4 and to determine concentration of given unknown solution.
- (b) Analysis of electronic spectrum of organic compounds

7. Photochemistry

- (a) To determine the quantum yield of chloride ion during the photolysis of an aqueous solution of Monochloroacetic acid by light of 253.7 nm wavelength.
- (b) To study photochemical bleaching of dyes (Methylene blue or malachite green) using a spectrophotometer.
- (c) To study photochemical decomposition of H_2O_2 .

8. Polarimetry

- (a) To study the inversion of cane sugar, a first order reaction with the help of a Polarimeter.
- (b) To determine optical rotation of different optically active substances.

9. Miscellaneous

- (a) To determine turbidity with the help of a turbidity meter.
- (b) To study conductometric titrations of a mixture of acid and base.
- (c) To study pH metric titrations of a mixture of acid and base.

REFERENCES:

1. *Practicals in Physical Chemistry*, P. S. Sindhu, MacMillan India Ltd, **2005**.
2. *Practical Physical Chemistry*, A. M. James and F. E. Prichard, Longman, **1974**.
3. *Findley's Practical Physical Chemistry*, B. P. Levitt, Longman, **1973**.
4. *Experiments in Physical Chemistry*, D. Shoemaker and C. W. Gasland, Tata Mc Graw
5. *Experimental Physical Chemistry*, G. P. Methewala, Glaredon Press, **1985**.
6. *Experimental Physical Chemistry*, R. C. Das and B. Bahera, Tata Mc Graw **1983**.

CY-592 Electronics for Chemists Lab

1. Study of Voltmeter, Current Meter and Oscilloscope
2. Study the performance of Half wave and full wave rectifiers
3. Study the performance of voltage regulator
4. Study the performance of Wein's Bridge Oscillator and RC phase shift oscillator
5. Study the performance of colpits and Hartley oscillator
6. Study the performance of inverting, non-inverting and units buffer
7. Study the performance of adder and subtractor circuits
8. Study the light intensity measurement circuit
9. Study of conductivity and pH of a liquid.
10. To get familiar with the working knowledge of the following instruments: (a) Cathode ray oscilloscope (CRO) (b) Multimeter (Analog and Digital) (c) Function Generator (d) Power supply and to measure phase difference between two wave forms using CRO(b) to measure an unknown frequency from Lissajous figures using CRO
11. (a) Plot the forward and reverse V-I characteristics of P-N junction diode (b) Calculation of cut-in voltage (c) Study of Zener diode in breakdown region.
12. To find frequency response of a given amplifier and calculate its bandwidth.
13. To get familiar with pin configuration of typical op-amp (741) and its use as: (a) Inverting amplifier (b) Non-inverting amplifier (c) Summing amplifier (d) Difference amplifier
14. Use of op-amp as (a) Integrator (b) Differentiator
15. To assemble Wein Bridge oscillator circuit and calculation of oscillation frequency and its verification from the observed output.
16. To assemble and test 5V/9 V DC regulated power supply and find its line-regulation and loaded regulation.
17. Verification of truth tables of logic gates (OR, AND, NOT, NAND, NOR)

REFERENCES:

1. *Practical Electricity and Electronics*, J. Watson, Macmillan Publication London, **1994**.
2. *Operational Amplifiers*, Gyekwad, Prentice Hall Publication, **1988**.

Prepared By: Dr. Arun Khosla
 Ratified By: Dr. R K Sarin

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| CY-597 | Summer Training (after second semester) | | 0 | 0 | 4 | 2 |
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Note : Summer Training is compulsory for M. Sc. 2nd year Students During Summer Vacations in some other Institutions / Industries like IITs , CSIR Labs , IOCL etc.

SEMESTER - III

INORGANIC PREPARATION

1. Preparation of Inorganic and Coordination compounds, their purification, elemental analyses, M.W determination and elucidation of structures by physical methods:

- Synthesis of Tris(acetylacetonato)manganese(III), $Mn(acac)_3$ and their characterization using magnetic susceptibility balance (MSB) and infra red spectroscopy (IR) (Green Preparation).
- Synthesis and Characterization of Hexamminechromium (III) nitrate $[Cr(NH_3)_6](NO_3)_3$ using magnetic susceptibility balance (MSB) and infra red spectroscopy IR (Green Preparation) .
- Synthesis of Iron(III) acetylacetonate and its characterization using magnetic susceptibility balance (MSB) and infra red spectroscopy (IR) .
- Synthesis and characterof nitro- and nitropentammincobalt (III) chlorides Using infra red spectroscopy (IR).
- Synthesis of hexamminecobalt(III) chloride and pentammineaquocobalt(III) chloride.
- Synthesis of cis- and trans- potassiumdioxalatodiaquochromate(III).
- Aquation of trans-dichlorobis(1,2-diaminoethane)cobalt(III) chloride.
- Synthesis and resolution of tris(ethylenediamine)cobalt(II) ion.
- Synthesis of Hexaamminenickle (II) chloride and estimation of Ni (II) in the complex by gravimetry and volumetry.
- Synthesis of tris(acetylacetonato)iron(III).
- Synthesis and reactivity of organocobaloximes.
- Synthesis of acetylferrocene and its purification by column chromatography.
- Synthesis of ferrocene carboxylic acid.

1. Qualitative Ion Exchange Technique:

- Separation of zinc and magnesium on an anion exchanger
- Separation of chloride and bromide on an anion exchanger
- Determination of the total cation concentration in water
- Separation of cadmium and zinc on an anion exchanger.

2. Complexometric Titrations:

- Determination of calcium in the presence of magnesium using EGTA as titrant.
- Determination of the total hardness (permanent and temporary) of water
- Determination of calcium in the presence of barium using CDTA as titrant.

3. Electro Analytical Techniques-pH metric, Conductometric and Amperometric Titration: Representative acid-base and redox titrations.

4. Colorimetry and Spectrophotometry:

- Determination of λ_{max} the absorption curve and concentration of a substance

- (b) Simultaneous spectrophotometric determination (chromium and manganese)
- (c) Spectrophotometric determination of pK value of an indicator
- (d) Determination of copper (II) with EDTA
- (e) Determination of iron (III) with EDTA.
- (f) Virtual Labs.

5. Atomic Absorption Spectroscopy:

- (a) Determination of cations by AAS
- (b) Determination of magnesium and calcium in tap water
- (c) Determination of trace elements in contaminated soil
- (d) Determination of vanadium in lubricating oil, determination of trace lead in a ferrous alloy.

6. Synthesis of Green Reagents:

- (a) Tetrabutylammonium tribromide (TBATB) and its application
- (b) Ionic Liquid, 1-methyl-3-pentyl-imidazolium bromide, [pmlm]Br and its application

7. Inorganic analysis by using green methods:

8. Qualitative determination by UV, IR, NMR, ESR:

REFERENCES:

1. Chemical Curiosities, H. Denny and W. Roesky, WILEY VCH, Ed. 1996.
2. Practical Inorganic Chemistry, G. Marr and B. W. Rocket, University Science Books, Ed. 1999.
3. Practical Inorganic Chemistry, G. Pass and H. Sutcliffe, Chapman and Hall, London, Ed. 1968.
4. Vogel's Textbook of Quantitative Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. Thomas, Pearson, Ed. 2006.
5. Vogel's Textbook of Quantitative Analysis, G. Svehla, Pearson, Ed. 2006.
6. A Collection of Interesting General Chemistry Experiments, Anil J. Elias, University Press, Ed. 2002.

Note: The students are required to perform at least 1 or 2 experiments from each section.

Prepared By: Dr. Sangeeta Obrai

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CY- 600

Project (Phase – I)

Note : It is compulsory for the M. Sc. Final year students to carry out minimum six month project / research work under the supervision of the faculty member.

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CY-611 Chemistry of Transition and Inner - Transition Elements

- 1. Survey of Transition Metal Chemistry** – Electronic configuration, general characteristics, oxidation states, pi-acid ligands, metal complexes, metal- *metal* bond, Quadruple bonds.
- 2. Chemistry of First Transition Series** – The elements, compounds, complexes, organometallics and bioinorganic chemistry of first transition series in different oxidation states .
- 3. Chemistry of Second & Third Transition Series** – The elements, compounds, complexes, organometallics and bioinorganic chemistry of second and third transition series in different oxidation states .
- 4. Lanthanides:** Electronic configuration, oxidation states, coordination numbers and stereochemistry, Magnetism and spectra, complexes and organometallic chemistry of lanthanides.
- 5. Actinides:** Electronic configuration, oxidation states, coordination numbers and stereochemistry, Magnetism and spectra, complexes and organometallic chemistry of Actinides.
- 6. Transition Metal Catalyzed Reactions:** Oxidative addition, Elimination reactions, Migration reactions.
- 7. Mechanism of Inorganic Reactions:** Inner sphere, Outer sphere, Trans effect.

REFERENCES:

- Inorganic Chemistry. 4th edition* D. F. Shriver and P. W. Atkins, Oxford University, Oxford, **2006**.
- Advanced Inorganic Chemistry* by F. A .Cotton and G .Wilkinson et al – Sixth edition, John Wiley & Sons, **2003**.
- Inorganic Chemistry* J. E. Huheey et al Fourth edition, Pearson, **2005**.
- Concepts & Model of Inorganic Chemistry* B. Douglas et. al, John Wiley & Sons, **2001**.
- Chemistry of elements*, N. N. Greenwood Pergamon Press, **2000**.
- Ligand Field Theory*, B. N. Figgis, Wiley Eastern, **1976**.

Prepared By: Dr. Sangeeta Obrai
 Checked By: Dr. S B S Mishra

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CY-621 Physical Methods of Structure Elucidation

- 1. Ultraviolet (UV) Spectroscopy:** Principles, origin, effect of structure, solvents, conjugation and Chromophore and Auxochromes, the Woodward-fieser rules, PES and related spectroscopy.
- 2. Microwave Spectroscopy:** Rotation of molecules and rotational spectra-Diatomic molecules, polyatomic molecules-Linear, symmetric top and asymmetric top molecules.
- 3. Infrared Spectroscopy:** Principle and instrumentation, Diatomic molecules-Energy of a diatomic molecule-simple harmonic oscillator-Anharmonic Oscillator- diatomic vibrating rotator, vibration-rotation spectrum of diatomic and polyatomic molecules-fundamental.
- 4. Raman Spectroscopy:** Raman scattering-Classical and Quantum theories of Raman Effect.
- 5. Mossbauer Spectroscopy:** Principles and applications of Mossbauer spectroscopy.
- 6. Magnetic Resonance Spectroscopy:** Magnetic resonance- spin angular momentum, Larmor frequency, Relaxation time, NMR spectroscopy of proton and C¹³Introduction to ESR. Hyperfine structure and double resonance in ESR. Applications of ESR spectroscopy.
- 7. Mass Spectroscopy:** Principles instrumentation and applications.

REFERENCES:

- Fundamental of Molecular Spectroscopy*, C. N. Banewell, 4th Edition, Tata Mc Graw-Hill Publication, **1995**.
- Introduction to Molecular Spectroscopy*, G. N. Barrow, Mc Graw Hill Publications, **1980**.
- Spectroscopic Methods in Organic Chemistry*, D. H. Williams and I. Flemings, Tata Mc Graw-Hill Publication, **1994**.
- Physical Method in Chemistry*, R. S. Drago, Sunders, **1985**.

Prepared By: Dr. Rajeev Jindal
Ratified By: Dr. N C Kothiyal
 Dr. B S Kaith
 Dr. Jaspreet Rajput

| L | T | P | C |
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CY-631 Analytical Principles and Instrumental Methods of Analysis

- Data Analysis:** Uncertainties, Errors, calibrations, Mean, Standard Deviation , Least square fit,
- Atomic Absorption Spectroscopy:** General principles, instrumental set up and analytical procedures and applications,
- Thermo-Analytical Method:** Theory, instrumental requirements and methodology for thermo gravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC), applications
- Chromatographic Methods:** Classification of chromatographic methods according to separation and development procedure, Instrumentation and applications (GC and HPLC)
- Electrochemical Techniques:** Conductometry, pH metry, Karl Fischer titration, cyclic voltametry ,Polarography
- Modern Methods of Surfaces and Crystal Analysis:** SEM, TEM, AFM, XRD

REFERENCES:

- Instrumental Methods of Analysis*, Willard, Merritt, Dean and Settle, CBS Publisher and Distributors.,**1986**.
- Thermal Analysis*, W. W. Wendlandt and L. W. Collins, Dowden Hutechin and Ross
- Basic Concepts of Analytical Chemistry*, S. M. Khopkar , Wiley Eastern
- Thermal Methods of Analysis*, Principles, Application and Problems, J. Haines, Blackie Academic and Professional, **1994**.
- Chromatographic Methods*, A. Braithwaite and F. J. Smith, 5th edn. Blackie Academic and Professional, London, **1996**.
- Principles of Instrumental Analysis*, Skoog, Holder, Nieman, Fifth edition Thomson Books ,**1998**.

Prepared By: Dr. N C Kothiyal
Ratified By: Dr. B S Kaith

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| CY-6XX | Elective – I | | 3 | 1 | 0 | 4 |
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SEMESTER – IV

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| CY-596 | Comprehensive Viva | L | T | P | C |
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| CY- 598 | Scientific Documentation and | L | T | P | C |
| | Presentation Skills | 0 | 0 | 2 | 1 |
| | (Exercises for scientific documentation & | | | | |
| | Presentation skills, Group Discussion etc) | | | | |

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| CY-599 | Seminar –II | L | T | P | C |
| | | 1 | 0 | 0 | 1 |

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| CY-600 | Project | L | T | P | C |
| | (Phase- II) | 0 | 0 | 16 | 8 |

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| CY- | Elective - II | L | T | P | C |
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| CY- | Elective – III | L | T | P | C |
| | | 3 | 1 | 0 | 4 |

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| CY- | Elective – IV | L | T | P | C |
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ELECTIVES

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CY-612 Natural Products

1. **Alkaloids:** Introduction, Nomenclature, Classification, Isolation, properties, Biosynthesis, Structure elucidation, Synthesis of some important types of alkaloids.
2. **Terpenoids:** Introduction, Classification, Isolation, Biosynthesis, Structure elucidation, Synthesis of some important types of terpenoids.
3. **Steroids:** Introduction, Classification, Isolation, Biosynthesis, Structure elucidation, some important types of steroids, Sex hormones (male and female), Adrenal cortisone hormone.
4. **Insects & Plant Growth Regulators:** Introduction, Hormones of endocrine system, Exocrine secretions, Plant growth regulators, Auxins, Gibberellins etc.
5. **Vitamins:** Introduction, Classification, Physical and chemical properties, Biological and physiological functions of Vitamin A, Vitamin B-complex, Vitamin C, Vitamin D, Vitamin K, Vitamin E and Vitamin H.
6. **Chemical analysis of phyto-constituents:** Preliminary and confirmatory chemical tests for Alkaloids, Terpenoids, Steroids, Sapogenins etc.

REFERENCES:

1. *Organic Chemistry*, Vol I-IV by Gilman, John Wiley & Sons, **1984**.
2. *Organic Chemistry*, Vol. II, I. L. Finar, Pearson Education, 6th edition, **2004**.
3. *The Alkaloids* by Monk and Holmes, Academic Press, **1990**.
4. *Steroids*-by Feiser and Feiser, Asia Publishing House, Bombay, **1980**.
5. *The Alkaloids* by Benty, Oxford University Press, **1974**.

Prepared By: Dr. B. S. Kaith
Ratified By: Dr. N. C. Kothiyal
Dr. Rajeev Jindal

L T P C
3 1 0 4

CY-622

Ligand Field Theory

1. **Introduction:** The concept and scope of Ligand Field Theory, Crystal Field & Ligand Fields, p & d orbitals.
2. **Quantitative Basics of Crystal Field:** Octahedral and Tetrahedral Crystal Field Potentials (V_{oct} & V_{tet}).
3. **Free Ions in Crystal Fields:** Effect of Cubic Crystal Fields on S,P,D,F,G,H & I Terms.
4. **Thermodynamic Aspects of Crystal Fields:** CFSE & its relation with lattice energy, Heat of Ligandation and Standard Electrode Potential.
5. **Electronic Spectra:** Spectra of ML_6^{n+} (spin free), ML_6^{n+} (spin paired), distorted octahedral and tetrahedral complexes, charge transfer bands, spectrochemical and nephelauxetic series.
6. **Magnetic Properties:** Magnetic properties of A, E & T Terms, E.S.R and magnetism.
7. **Non Cubic Symmetry:** Square Planar, Square pyramidal and dodecahedral coordination compounds.

REFERENCES:

1. *Introduction to Ligand Fields*, B. N. Figgis, Wiley Eastern, **1976**.
2. *Chemical Applications of Group Theory*, F. A. Cotton, Wiley, **1996**.
3. *Physical Inorganic Chemistry*, S. F. A. Kettle, Oxford, **1998**.
4. *Ligand Field Theory & Its Applications*, B. N. Figgis & M. A. Hitchman, Wiley, **2000**.
5. *Inorganic Electronic Spectroscopy*, A. B. P. Lever Elsevier, **1984**.

Prepared By: Dr. Sangeeta Obrai
Ratified By: Dr. S B S Mishra

L T P C
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CY-623

Polymer Chemistry

1. **Introduction:** Basic concepts, nomenclature, tacticity, Effects of polymer structure on its physical, chemical and mechanical properties. Functionality and its role in determining the properties of a polymer, various methods for the determination of molecular weights.
2. **Polymerization Techniques:** Types of polymerization and their mechanisms i.e. free radical, cationic, anionic and co-ordination polymerization and their applications in different fields.
3. **Molding Techniques:** Introduction, different molding techniques (both for Thermosetting and thermoplastic resins), additives and their functions, applications of different molding techniques.
4. **Conducting Polymers:** Introduction, classification, different types of dopings, synthesis, applications in different fields.
5. **Composites:** Introduction, classification, different types of reinforcing materials and their applications, failure modes, advantages and applications.
6. **Biopolymers:** Introduction, types and their applications as bio-composites, Sustained drug delivery devices and in water treatment technology, controlled release of nutrients, water and insecticides / pesticides to plants.

REFERENCES:

1. Text book of Polymer Sciences, F. W. Billmeyer, Jr. Wiley-Intersciences, 3rd Ed. 1984.
2. Polymer Chemistry, Basic concepts, Paul C. Hiemanz, Marcel Dekker, Ed. 1984.
3. Organic Polymer Chemistry, K. J. Saunders, Chapman and Hall, London, 2nd Ed. 1988.
4. Principles of Polymer Chemistry, P. J. Flory, Cornell Univ. Press, Ithace, Ed. 1953.
5. Polymer Science and Technology, Plastics, Rubbers, Blends and Composites, Premamoy Ghosh, Tata McGraw-Hill, 2nd Ed. 2002.

Prepared By: Dr. B. S. Kaith

CY-632

Bioinorganic Chemistry

- Enzymes** : Introduction and historical prospective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fisher's lock and key and Koshland's induced fit hypothesis, concept and identification of active sites by the use inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.
- Mechanism of Enzyme Action** : Transition state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, Examples of some typical enzyme mechanism for chymotrysin, ribonuclease, lysozyme and carboxypeptidase A.
- Metal Ions in Biological Systems** : Essential and trace metals.
- Na⁺/K⁺ Pump** : Role of metal ions in biological processes.
- Bioenergetics and ATP Cycle** : DNA polymerization, glucose storage, metal complexes in transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water model system.
- Transport and storage of Dioxygen** : Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.
- Electron Transfer in Biology** : Structure and function of metalloproteins in electron transport processes- cytochromes and iron-sulphur proteins, synthetic models.
- Nitrogenase** : Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

REFERENCES:

- The Biological Chemistry of the Elements*, J. R. Frausto & R. J. P. Williams, Oxford University Press, **2001**.
- Bioinorganic Catalysis*, Reedijk & E Bouwman (ed), Marcel & Dekker, **1999**.
- Molecular to Global Photosynthesis*, M. D. Archer & J. Barder (ed), Imperial College Press, **2004**.
- Inorganic Aspects of Biological and Organic Chemistry*, R. P. Hanzbk, Academic Press New York, **1978**.
- Bioorganic Chemistry*, E . I. Allyn & B. Boston, **1977**.

Prepared By: Dr. Rajeev Jindal
 Ratified By: Dr. B S Kaith

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CY - 633 Advanced Inorganic Chemistry – I

- 1. Principles :** Molecular Structure and Bonding. A review of Lewis Structures including Formal Charges and VSEPR model. Molecular orbital theory of homo- and heteronuclear diatomic molecules. M.O theory of solids, Periodicity and related concepts, Chemical Forces.
- 2. Oxidation and Reduction:** Reduction Potentials, Redox Stability in water , diagrammatic presentation of potential data , acids and bases, Various definitions including HSAB principles.
- 3. Solid-state :** Close-packing of Solids, types and structures of Ionic Solids; radius ratio rules; Lattice Energy; Born –Haber Cycles, Defects in Solids and properties of solids arising out of defect structures, Perovskite Structures, High T_c Superconductors.
- 4. Ligands and complexes :** Various types of ligands, Structure and isomerism in complexes.
- 5. Bonding and electronic spectra :** Valence Bond-, Crystal Field – and Molecular Orbital Theories of Complexes, Preliminary ideas on Electronic Spectra and Magnetism of Transition metal complexes.
- 6. Organometallic chemistry :** Introduction to Organometallic Chemistry, ideas on M-C bond; Ligands involved, electron count. Some examples of organometallic compounds.
- 7. Metal ions in medicine and materials :** Introduction to the role of metal ions in medicine and materials : preliminary ideas on bio-Inorganic Chemistry, Oxygen transport and storage, cytochrome P_{450} , cytochrome c , metallo enzymes.

REFERENCES:

1. *Inorganic Chemistry 4th edition* D. F. Shriver and P. W. Atkins, Oxford University, Oxford, **2006**.
2. *Inorganic Chemistry*, J. E. Huheey et al, Fourth edition, Pearson, **2005**.
3. *Concepts & Model of Inorganic Chemistry*, B. Douglas et al, 3rd John Wiley & Sons, **2001**.
4. *Chemistry of elements*, N. N. Greenwood Pergamon Press, **2000**.
5. *Ligand Field Theory*, B. N. Figgis, Wiley Eastern, **1976**.

Prepared By: Dr. Sangeeta Obrai
Ratified By: Dr. S B S Mishra

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CY – 634

Advanced Inorganic Chemistry – II

- 1. Coordination Chemistry** : Coordination number and structures of coordination complexes. Theory of bonding, crystal field and molecule orbital theory. JT distortion Electronic Spectra of coordination compounds. Tanabe-Sugano diagrams, Stereochemistry of non-rigid and fluxional molecules. Thermodynamic aspects of coordination complexes : Irving William Series. Kinetic aspects : reactions and aquation rates, electron transfer reactions. Reaction mechanism in inorganic reactions. Redox reactions.
- 2. Organometallic Chemistry** : Structure, Bonding and Reactivity studies of metal carbonyls, nitrosyls, dinitrogen complexes, metal alkyls, carbenes, carbenes and carbides. Metallocenes and related chemistry. Homogeneous and heterogeneous catalysis. Organometallic complexes with metal-metal bonds.
- 3. Supramolecular Chemistry** : Pederson's crown ether, Cram's principle of preorganization, Lehn's Cryptands. Covalent and non-covalent forces. Principle of self-assembly . Host guest chemistry and molecular receptors. Supramolecular inorganic architectures. Supramolecular photochemistry, transport process and carrier design.
- 4. Molecular Magnetism** : Fundamental equations in molecular magnetism, magnetic susceptibility, orbital quenching and spin-only moment. Magnetic exchange interactions in multinuclear coordination compounds. Low spin high spin transition, intermediate spin and spin admixed states. Molecule –based magnetic materials.
- 5. Inorganic Chemistry of Biological Systems** : Energy sources for life, metalloprophyrins, dioxygen binding, transport, utilization, electron transfer, photosynthesis, nitrogen fixation, essential and trace elements in biological systems, biochemistry of non-metals.
- 6. Inorganic compounds in medicine and materials** : Metal complexes in organic reactions, cisplatin, gold complexes, technetium complexes, metal nano-particles in heterogeneous catalysis, metal embedded polymers as functional materials, metal complexes in display technologies, Inorganic vapochromic materials, molecule-based magnetic materials. DNA cleavage by transition metal complexes, anti-cancer drugs, therapeutic drugs, metal and non-metals in PET.

REFERENCES:

- Inorganic Chemistry 4th edition* D. F. Shriver and P. W. Atkins, Oxford University, Oxford, **2006**.
- Inorganic Chemistry – Principles of Structure and Reactivity. 4th Edn.* J.E. Huheey, E. A. Keiter and R.L. Keiter Harper-Collins, NY, **1993**.
- Modern Inorganic Chemistry. 2nd Edn.* W.L. Jolly, McGraw-Hill, Singapore, **1991**.
- Concepts and Models of Inorganic Chemistry. 3rd Edn.* B. Douglas, D. Mc Daniel, and J. Alexander, John Wiley, New York. **1993**.
- Molecular Magnetism.* O. Kahn, VCH, Weinheim, **1993**.
- Supramolecular Chemistry.* J. M. Lehn, VCH, Weinheim, **1995**.

Prepared By: Dr. Sangeeta Obrai

Ratified By: Dr. S B S Mishra

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CY -641

Solid State Chemistry

- 1. Electronic structure of solids** : Introduction, Simple non-metallic solids, Transition metal compounds, Defects and impurities.
- 2. Chain compounds and one dimensional physical behaviour** : Introduction. Special features of chain compounds, Structures of chain compounds, Physical properties of chain compounds.
- 3. Superconducting Materials** : Introduction, General properties of semiconductors, Critical temperature, Qualitative features of microscopic theory of superconductivity, Basics ideas of BCS theory, , the zero resistance phenomenon , Superconductivity and magnetism.
- 4. Catalysis** : Homogeneous catalysis by transition metal complexes : Hydrogenation reactions with early transition metals and lanthanide catalysis, Hydroformylation reactions, Heterogeneous catalysis : Mechanistic features, Chemisorption, Desorption, Multimetallic catalysts.
- 5. Zeolite** : Introduction, Structures, compositions, Geological occurrence, Zeolite synthesis, Aluminosilicate gel, Crystalline mechanisms, Zeolites as ion exchangers, Zeolite catalysts, Interconversion of aromatics by Zeolites, Towards the future, Clays, pillared clays, and layered double hydroxides.
- 6. Ferroics** : Introduction, Proper and Improper ferroics, Primary and secondary Ferroics, Ferroelectrics, Relaxor ferroics.

REFERENCES:

1. *Solid State Chemistry-Compounds*, A. K. Cheetam, P. Day, Oxford, **2001**.
2. *Solid State chemistry-An Introduction*, Lesley smart, Elaine Moore, Nelson Thomas ltd, **2001**.
3. *Basic Solid State Chemistry*, A. R. West, Wiley, **1999**.
4. *Solid State Chemistry & Its Applications*, A. R. West, John Wiley & Sons, **2003**.
5. *Structural Inorganic Chemistry*, A. F. Wells, Oxford, **1985**.
6. *Inorganic Structural Chemistry* U. Muller, Wiley, **1993**.

Prepared By: Dr. Sangeeta Obrai
Ratified By: Dr. S B S Mishra

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CY- 650

Nanochemistry

- 1. Nanochemistry Basics:** Nanochemistry, self assembly, Self assembling materials, two dimensional assemblies, Mesoscale self assembly, coercing colloids.
- 2. Chemical Patterning, Lithography & Nanocontact Printing:** Soft lithography, Microlens arrays, Nonoring arrays, SAM crystal engineering, Sweet chips, Dip pen nanolithography, Nanoplotters, Nanoblotters,
- 3. Nanorod, Nanotube, Nanowire Self- Assembly:** Templating nanowires, nanorods, Nanorod devices, Nanowire sensors, diodes & transistors.
- 4. Carbon nanostructures:** Carbon molecules, clusters, carbon nanotubes and their applications.
- 5. Organic Compounds and Polymers:** Nanocrystals, polymers, Supromolecular structures
- 6. Scope and opportunities:** Nanoscale materials, nanotechnology enabled sensors, microelectronics, drug delivery, Bionanoinformation.

REFERENCES:

1. *Nanochemistry, A Chemical approach to Nanomaterials*, G. A. Ozin & Andre, C. Arsenault, Royal society of Chemists, **2005**.
2. *Introduction to Nanotechnology*, C. P. Poole, Jr., F. J. Owens, Wiley interscience, **2003**.
3. *Nanotechnology, Science Innovation & Opportunity*, L. E. Foster, Pearson Education, **2007**.

Prepared By: - Dr. Jaspreet Rajput
Ratified By: - Dr. S B S Mishra

CY-651 Photochemistry

- 1. Photochemical Reactions :** Interaction of electromagnetic radiation with matter, types of excitations, rate of excited molecule, quantum yield, transfer of excitation energy, actinometry, photochemical laws, flash photolysis, stopped flow techniques, energy dissipation by radiation and non-radiative processes, Franck-condon principle, photochemical stages-primary and secondary process.
- 2. Determination of Reaction Mechanism :** Classifications, rate of 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 :** Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.
- 4. Photochemistry of Carbonyl Compounds :** Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic, β , γ -unsaturated and α,β -unsaturated compounds. Cyclohexadienones. Intermolecular cycloaddition reactions- dimerisation and oxetane formation.
- 5. Photochemistry of Aromatic Compounds:** Isomerisation, additions and substitutions.
- 6. Miscellaneous Photochemical Reactions :** Photo-Fries reactions of anilides, Photo-fries rearrangement. Barton reaction, singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.
- 7. Inorganic Photochemical Processes:** Photosubstitution, rearrangement and redox reactions.

REFERENCES:

1. *Fundamentals of Photochemistry*, K. K. Rohtagi-Mukherjee, Wiley Eastern Ltd., **1986**.
2. *Excited States in Organic Chemistry*, J. A. Baltrop and J. D. John Wiley, **1975**.
3. *Aspects of Organic Photochemistry*, W. M. Horspol, Academic Press, **1976**.
4. *Molecular Reactions and Photochemistry*, C. H. Depuy and O. S. Chapman, Prentice Hall of India, **1988**.
5. *Modern Molecular Photochemistry*, N. J. Turro, Benjamin Cumming Publishing co. Inc., **1978**.

Prepared By: Dr. Rajeev Jindal
 Ratified By: Dr. B S Kaith

CY- 653

Statistical Thermodynamics

- 1. Generalized Coordinates of Phase Space:** Phase Space, density distribution in phase space, Liouville's Theorem, Microcanonical ensemble, Postulates of equal probabilities
- 2. The Classical Distribution Law:** Maxwell's Boltzmann Distribution Law, Maxwell's law of distribution of velocities, Principle of Equipartition of Energy
- 3. Introduction to Quantum Statistics:** Bose Einstein Statistics, Fermi Dirac Statistics, Maxwell Boltzmann Statistics, comparison of Bose Einstein, Fermi Dirac and Maxwell Boltzmann Statistics
- 4. Thermodynamics and Statistics:** Entropy and Probability, Entropy and number of eigen states, Thermodynamics of a Monoatomic Gas
- 5. Partition Function:** Partition function and Thermodynamic Properties, Translational Partition Function, Sackur-Tatode Equation, Separation of Internal Partition Function, rotational and Vibrational Partition Function
- 6. Applications of Partition Function:** Determination of thermodynamic properties, Ortho and Para hydrogen, free energy functions, Equilibrium Constant, effect of nuclear spin, Isomolecular reactions
- 7. Non-equilibrium Thermodynamics:** General Theory of non-equilibrium thermodynamics, entropy production in heat flow, matter flow and electric current, Onsager's reciprocal relations

REFERENCES:

1. *Physical Chemistry*, P. Atkins, J. D. Paula, Indian Edition, Oxford, **2007**.
2. *Thermodynamics, Statistical Thermodynamics, and Kinetics*, T. Engel and P. Reid, Prentice Hall, **2006**.
3. *Thermodynamics, A Core Course 3rd Edition* R. C. Srivastava, S. K. Saha, A. K. Jain, Prentice Hall of India, **2007**.
4. *Physical Chemistry*, T. Engel and P. Reid, Prentice Hall, **2006**.
5. *Theoretical Chemistry*, Samuel Glasstone, Wiley
6. *Non-equilibrium Thermodynamics, Principles and Applications* C. Kalidas, M. V. Sangaranarayanan Macmillan India Ltd., **2002**.

Prepared By: Dr. Harsh Kumar
 Ratified By: Dr. Rajeev Jindal

L T P C
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CY-661 Nanomaterials, Nanoscience & Nanotechnology

1. **Introduction:** Terminologies, History & Scope.
2. **Characterization & Fabrication:** Contemporary Characterization Methods, Top down & Bottom up Fabrication, Solution based Synthesis of Nanoparticles, Vapour Phase Synthesis & Synthesis with framework, Nanolithography, Dip Pen Lithography.
3. **Artificially Layered Materials:** Quantum Well, Quantum Dots, Super lattices & Layered Structures.
4. **Self Assembly:** Supramolecular & Dimension Control in Nanostructure, thermodynamic and coded self assembly.
5. **Biomaterials:** DNA & Nanomaterials, Bionanocomposites, Biometrics, molecular motors.
6. **Nanoelectronics and Molecular Computing:** Molecular wires, Nanowires, Nanotubes, Molecular switch, Molecular logic gates and molecular storage devices, DNA Computing Quantum Computing.

REFERENCES:

1. *Introduction to Nanotechnology*, C. P. Poole & F. J. Owens, Wiley, **2003**.
2. *Understanding Nanotechnology*, Scientific American, **2002**.
3. *Nanotechnology*, M. Ratner & D. Ratner, Prentice Hall, **2003**.
4. *Nanotechnology*, M. Wilson, K. Kannagara, G. Smith, M. Simmons & B. Raguse, CRC Press Boca Raton, **2002**.

Prepared By: Dr. S B S Mishra
Ratified By: Dr. Jaspreet Rajput

L T P C
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CY-662 Industrial Organic Chemistry

1. **Synthetic Dyes:** Introduction, Structural Features, Uses, Classification as per chemical constitution, Colour and constitution, classification based on application, Nitro, Nitroso, Azo, Acid, Basic, Direct, Mordant, xanthenes, Heterocyclic and Sulphur dyes.
2. **Insecticides:** Brief Introduction and classification of insecticides and pesticides, chemical control of insects, Environmental friendly insecticides, uses and limitations.
3. **Synthetic Polymers:** Introduction and uses of synthetic rubbers, plastics and fibers, conducting polymers, polymers in electronic industries.
4. **Synthetic Detergents:** Introduction, classification chemistry and applications, additives for detergents, detergent and their Applications in Petroleum Industry.
5. **Explosives:** Introduction, Classification, Chemistry and Uses of Molecular and Emulsion Explosives.
6. **Synthetic Perfumes:** Introduction, chemistry and uses.
7. **Synthetic Drugs:** Introduction, Mechanism and drug action, Physiological activity and structures, Antimalarials, Sulpha Drugs, Metallic Therapeutics, Sweetening Agents.

REFERENCES:

1. *Chemistry of Antibiotics used in Medicine*, R. M. Evans, Pergman Press London **1969**.
2. *Steroids* by Fieser and Fieser, Asia Publishing House **1980**.
3. *The Vitamins-Chemistry*, Physiology, Pathology, Methods, Vol. 1 to 5 Sebrell Jr and R. S. Horis, Academic Press **1968**.
4. *Chemistry of Insecticides*, D. H. R. Barton and T. R. Roberts, Wiley Interscience Publications **1985**.
5. *Chemistry of Pesticides* K. H. Buchel John Wiley & Sons **1983**.

Prepared by – Dr. N. C. Kothiyal
Ratified by – 1. Dr. B. S. Kaith
2. Dr. Rajeev Jindal
3. Dr. Jaspreet Rajput

L T P C
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CY-665

Leather Chemicals

- 1. Polymer Fundamentals:** Concept of a macromolecule, natural and synthetic polymers
- 2. Modes of polymerization:** radical, condensation and stereo regular polymerizations, anionic and cationic polymerization, polymerization kinetics, , bulk, solution, suspension and emulsion polymerization.
- 3. Types of Polymers:** Polymers with linear, branched and cross-linked structures, thermoplastic and thermoset polymers.
- 4. Molecular weight and distribution of polymers:** different methods of molecular weight determinations, colligative properties, viscometry, light scattering techniques
- 5. Characterization of leather polymers:** TGA, DTA, DTG, XRD, FT-IR, SEM, TEM and DSC
- 6. Polymers for leather processing:** Introduction, syntans, filling agents, base coats, top coats and adhesives, manufacture of industrially important polymers for plastics, fibres and elastomers, Polyethylene, polypropylene, polyvinyl chloride, polyvinyl alcohol, polyacrylonitrile, polystyrene, polyurethane, fluoro-carbon polymers, epoxy, resins, polyamides, polyesters, alkyl resins, silicon polymers, cellulose, Natural rubber processing and vulcanizing
- 7. Fabrication of polymeric material:** compounding and mixing, casting , extrusion, fibre spinning, molding, coating and foam fabrication.
- 8. Leather Lubrication:** Chemistry of vegetable tannins, extraction of vegetable tannins, solid-liquid ratio for extraction, chemical modification and blending of vegetable tannins, importance of free oil to emulsifier ratio, Theory of leather lubrication
- 9. Dyes, pigments and colourants:** Colour measurement techniques, factors influencing fastness properties of dyes, pigments and colouring substances, finishing auxiliaries and importance of surface feel modification, role of slip agents, fillers, matting agents. Protein preservatives, role and function of hydrophobicity/hydrophilicity in preservation.

REFERENCES:

1. Treatise on Coatings, R. R. Myers, and J. S. Long, Marcel Dekker, Ed. 1975.
2. Acrylics and Their Uses in Leather Manufacture, S. Rajadurai and S. Kulasekaran, CLRI, Madras, Ed. 1982.
3. Polymer Science & Engineering, D. J. Williams, Prentice Hall, Ed. 1971.
4. Chemical Process Industries, G. T. Austin, McGraw-Hill International Book Co., 5th Ed. 1984.
5. Science & Technology of Rubber, F. R. Elrich, Academic Press, New York, Ed. 1978.

Prepared By: Dr B S Kaith

L T P C
3 1 0 4

CY-671 Drug Design and Development

1. **Drug Design: A Rational Approach:** Introduction-analogues and prodrugs – concept of “lead” , Quantum mechanical approach, Molecular orbital approach, Molecular connectivity approach, General considerations-tailoring of drugs.
2. **Drug Design and Development:** Screening of natural products-Isolation and purification-structure determination, structure activity relationships
3. **Cimetidine: A Rational Approach to Drug Design:** Introduction, biological activity, metabolism, conformational isomers
4. **Quantitative Structure-Activity Relationships (QSAR):** Introduction, Hydrophobicity, Electronic effects, Steric factors, physicochemical parameters
5. **Structural Features and Pharmacological Activity:** The influence of steric factors, optical, geometrical isomerism, conformational isomerism and pharmacological activity.
6. **Combinatorial Synthesis-The design of compound libraries and their application to drug discovery:** application, combinatorial chemistry, future development and lead optimization, design based on structural information.
7. **Computer Assisted Molecular Modeling in Rational Drug Design**

REFERENCES:

1. *An introduction to Medicinal Chemistry-Graham L. Patrik*, Oxford University Press, 3rd edition, **2005**.
2. *Medicinal Chemistry Vol-I & II –Burger*, Wiley-Inter Science, Division of John Wiley & Sons, New York, 5th edition, **1994**.
3. *Pharmaceutical Process Validation*, I. R. Berry & R. A. Nash, Academic Press, London, 3rd Edition, **2003**.
4. *The Organic Chemistry of Drug Design and Drug Action*, R. B. Silverman, Academic Press Inc. London , 2nd Edition, **2004**.

Prepared By: Dr. Jaspreet Rajput
Ratified By: Dr. N C Kothiyal

L T P C
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CY-681

Mechanistic Inorganic Chemistry

1. **Ligand Substitution** : Thermodynamic & Kinetic Aspects, Classification of Mechanisms.
2. **Ligand substitution in Square Planar Environment** : Nucleophilicity shape of transition state, examples.
3. **Ligand Substitution in Octahedral Environment** : Rate Laws, Activation, Stereochemistry and Isomerisation.
4. **Redox Reactions** : Classification, Inner sphere & Outer sphere mechanisms.
5. **Photochemical Reactions** : Prompt & delayed reactions metal-metal bond systems, d-d & charge transfer reactions.
6. **Catalysis** : Heterogeneous, Homogeneous catalysis and their important consequences.

REFERENCES :

1. *Inorganic Reaction Mechanism*, M. L. Tobe & J. Burgess, Longman, **1999**.
2. *Kinetics & Mechanism of Reactions of Transition Metals Complexes*, VCH, **1991**.
3. *Redox Mechanism in Inorganic Chemistry*, A. G. Lappin, E. Horwood , **1994**.
4. *Coordination Chemistry Reviews*, 249, **2005**.
5. *Mechanisms of Inorganic Chemistry*, F. Basolo and R. G. Pearson Wiley, **1967**.

Prepared By: Dr. Sangeeta Obrai
Ratified By: Dr. S B S Mishra

B. Tech Syllabus

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CY – 101

Chemistry

- 1. Solid State and Distribution Law:** Introduction to Solid State Chemistry, Law of rational indices, Miller indices, Interplaner spacing, X-ray diffraction, Nernst distribution law, Applications of distribution law: solvent extraction.
- 2. Chemical and Phase Equilibria:** Phase diagram for single component system, carbon dioxide system, sulphur system, carbon system, helium system, Two component systems: Pb-Ag system, Bi-Cd system, KI-H₂O system, Freezing mixtures, Azeotropic mixtures, solubility of partially miscible liquids.
- 3. Spectroscopic Studies of Materials:** Lambert-Beer's Law, Principles and applications of U. V. Visible, Molecular Absorption Spectroscopy, Chromophores, Effect of conjugation on chromophores, Absorption by aromatic systems, Rotational and Vibrational spectroscopy: Principles and application to simple molecules, Magnetic Resonance Spectroscopy: Principles and application to simple molecules and Introduction to Photoelectron Spectroscopy.
- 4. Organic Reactions and Reagents:** Oxidation of hydrocarbons, Oxidation of alcohols (chromic acid), oxidation of carbon-carbon double bonds (sharpless epoxidation) including Palladium-catalyzed oxidation, oxidation of ketones (Baeyer-Villiger oxidation). Catalytic hydrogenation, homogeneous hydrogenation (Wilkinson's catalyst), Reduction by dissolving metals (Birch reduction), Reduction by hydride-transfer reagents (NaBH₄), Reduction with boranes (BF₃).
- 5. Coordination Complexes:** Crystal field theory of octahedral and tetrahedral complexes, Spectrochemical series, High spin and low spin complexes. Charge transfer spectra, John- Teller effect, colour & magnetic properties.
- 6. Biological Inorganic Chemistry:** Oxygen transport and storage-Myoglobin, Hemoglobin, The chemistry of elements in medicine – chelation therapy, Cancer treatment, Anti-arthritis drugs, contributions of individual elements to biological systems.
- 7. Nano-science and Technology:** Introduction to Nano-science and technology, Self Assembly, Lithography, Soft Lithography, Dip pen nanolithography, CNTs, bio-nanoinformation, Applications in microelectronics.
- 8. Conducting Polymers:** Introduction, types, n-doping, p-doping, some specific examples of conducting polymers, conducting polymers – a comparison between metals and CPs, applications in diversified fields.

REFERENCES:

1. *Advanced Inorganic Chemistry* (6th edition), F. A. Cotton and G. Wilkinson, John Wiley and Sons, **2003**.
2. *Inorganic Chemistry* (4th edition), D. F. Shriver and P. W. Atkins, Oxford University, Oxford, **2006**.
3. *Modern methods of organic synthesis* (3rd edition), W. Carruthers, Cambridge University Press (Cambridge Low Price editions) 1986, Reprinted **2004**.
4. *Reactions, Rearrangements and Reagents* (4th edition), S. N. Sanyal, Bharti Bhawan (P & D), **2003**.
5. *Polymer Science and technology* (2nd Edition), P. Ghosh, Tata McGRAW Hill, **2008**.
6. *Applications of Absorption Spectroscopy of Organic Compounds* (4th edition), John R. Dyer, Prentice Hall of India Pvt. Ltd., **1978**.
7. *Introduction to Nanotechnology* , C. P. Poole Jr. , F. J. Owens, Wiley Interscience, **2003**.
8. *Nanotechnology Science, Innovation and Opportunity*, L. E. Foster, Pearson Education, **2007**.
9. *Spectroscopic methods in organic chemistry* (4th Edition), Williams & Fleming, Tata McGRAW Hill, **2003**.

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CY – 102 Chemistry Laboratory

1. To draw the phase diagram of lead-in binary system.
2. To study the adsorption of acetic acid on activated charcoal.
3. To verify Beer's law for a coloured solution and to determine the concentration of a given unknown solution.
4. Determine the partition coefficient of iodine between carbon tetrachloride and water.
5. Determine the viscosity of a given liquid by Oswald's viscometer.
6. To determine the molecular weight of a given compound by cryoscopy.
7. Isolation of caffeine from tea leaves.
8. To synthesize paracetamol and determine percentage yield of the product.
9. To synthesize Phenol and Urea formaldehyde resin.
10. Thin layer-chromatographic separations of amino acids / organic molecules.
11. Determination of ion-exchange capacity of a given ion-exchange (cationic / Anionic).
12. Determination of COD of water sample.
13. To draw the pH-titration curve of strong acid vs strong base.
14. To determine concentration of trace metals by atomic absorption spectrophotometer.
15. An investigatory project (compulsory for all students).

List of Open
Elective Courses for
B. Tech Students

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CY- 583 Molecular Electronic Devices

- 1. Introduction:** Background, Justification and prospects.
- 2. Molecular electronic Devices:** Advantage of molecules as electronic devices molecular design and constrains of molecular devices.
- 3. Molecular Wires:** Synthetic routes to design of molecular wire and their testing.
- 4. Molecular switches:** Alternative switching methodologies, molecules as switches.
- 5. Molecular Logic Gates:** Strengths of molecules as logic gates, examples of molecular logic gates and their applications.
- 6. Molecular Storage and Transport:** Design of molecules for storage and transport, methodologies and limitations.
- 7. Molecular Superconductors:** Molecular approach towards superconductivity, molecular magnetism and their correlation.
- 8. Quantum Computers:** Molecular approach towards computing, quantum computing, DNA computing and their limitations.

REFERENCES :

1. Molecular Electronics Vol. I & II, Ari Aviram, M. A. Ratnar and Vlademiro Mujica, Academy of Sciences, Ed. 2002.
2. Molecular Electronic-Commercial Insights, Chemistry, Devices, Architecture and Programming, James M. Tour, World Scientific, Ed. 2003.
3. Molecular Eelectronics, IUPAC- Chemistry for 21st Century Monographs, J. Jortner and M. Ratnr, Blackwell Science, Ed. 1997.
4. Organic Conductors-Super conductors and Magnets from Synthesis to Molecular Electronics, Lahcene Ouahab, Klumer Acad. Publisher, Ed. 2004.
5. Molecular Electronics, Synthesis & Testing of Components, J. M. Tour, Accounts of Chemical Research 33, 791-804, 2000.

Prepared By: Dr S B S Mishra

L T P C
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CY-623

Polymer Chemistry

1. **Introduction:** Basic concepts, nomenclature, tacticity, Effects of polymer structure on its physical, chemical and mechanical properties. Functionality and its role in determining the properties of a polymer, various methods for the determination of molecular weights.
2. **Polymerization Techniques:** Types of polymerization and their mechanisms i.e. free radical, cationic, anionic and co-ordination polymerization and their applications in different fields.
3. **Molding Techniques:** Introduction, different molding techniques (both for Thermosetting and thermoplastic resins), additives and their functions, applications of different molding techniques.
6. **Conducting Polymers:** Introduction, classification, different types of dopings, synthesis, applications in different fields.
7. **Composites:** Introduction, classification, different types of reinforcing materials and their applications, failure modes, advantages and applications.
6. **Biopolymers:** Introduction, types and their applications as bio-composites, Sustained drug delivery devices and in water treatment technology, controlled release of nutrients, water and insecticides / pesticides to plants.

REFERENCES:

6. Text book of Polymer Sciences, F. W. Billmeyer, Jr. Wiley-Intersciences, 3rd Ed. 1984.
7. Polymer Chemistry, Basic concepts, Paul C. Hiemanz, Marcel Dekker, Ed. 1984.
8. Organic Polymer Chemistry, K. J. Saunders, Chapman and Hall, London, 2nd Ed. 1988.
9. Principles of Polymer Chemistry, P. J. Flory, Cornell Univ. Press, Ithace, Ed. 1953.
10. Polymer Science and Technology, Plastics, Rubbers, Blends and Composites, Premamoy Ghosh, Tata McGraw-Hill, 2nd Ed. 2002.

Prepared By: Dr. B. S. Kaith

L T P C
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CY-661 Nanomaterials, Nanoscience & Nanotechnology

1. **Introduction:** Terminologies, History & Scope.
2. **Characterization & Fabrication:** Contemporary Characterization Methods, Top down & Bottom up Fabrication, Solution based Synthesis of Nanoparticles, Vapour Phase Synthesis & Synthesis with framework, Nanolithography, Dip Pen Lithography.
3. **Artificially Layered Materials:** Quantum Well, Quantum Dots, Super lattices & Layered Structures.
4. **Self Assembly:** Supramolecular & Dimension Control in Nanostructure, thermodynamic and coded self assembly.
5. **Biomaterials:** DNA & Nanomaterials, Bionanocomposites, Biometrics, molecular motors.
6. **Nanoelectronics and Molecular Computing:** Molecular wires, Nanowires, Nanotubes, Molecular switch, Molecular logic gates and molecular storage devices, DNA Computing Quantum Computing.

REFERENCES:

1. *Introduction to Nanotechnology*, C. P. Poole & F. J. Owens, Wiley, **2003**.
2. *Understanding Nanotechnology*, Scientific American, **2002**.
3. *Nanotechnology*, M. Ratner & D. Ratner, Prentice Hall, **2003**.
4. *Nanotechnology*, M. Wilson, K. Kannagara, G. Smith, M. Simmons & B. Raguse, CRC Press Boca Raton, **2002**.

Prepared By: Dr. S B S Mishra
Ratified By: Dr. Jaspreet Rajput

List of Courses
Exclusively for Ph D
Chemistry Students

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CY-761 Principles of Instrumental Methods of Analysis

- 1. Data Handling** : *Introduction ,Sensitivity and Detection limit, Noise and sources, Uncertainties, Errors, calibrations, Mean, Standard Deviation , Least square fit, computer aided analysis*
- 2. Thermo Analysis** : *Basic principle ,Instrumentation and working of thermo gravimetric analysis (TGA), differential thermal analysis DTA (or DSC) and TG, applications of thermal analysis ,Thermometric titrations*
- 3. Gas Chromatography** : *Classification of chromatographic methods, Principles of Gas Chromatography, plate theory, Instrumentation, Working, Applications, Gas Solid Chromatography*
- 4. High Performance Liquid Chromatography** : *Principle, Instrumentation, Supports in HPLC, Applications of HPLC systems, Supercritical fluid Chromatography (SFC), Recent developments in SFC and Applications*
- 5. Exclusion Chromatography** : *Gel permeation Chromatography, Applications of GPC, Ion Exclusion, Mechanism of ion exclusion technique.*
- 6. Atomic Absorption Spectroscopy** : *General principles, instrumental for AAS and analytical procedures, sensitivity and detection limit in analysis, applications.*
- 7. Electrochemical Techniques** : *Basic principle ,Instrumentation and applications of cyclic voltametry and Polarography*
- 8. Modern Methods of Surfaces Analysis** : *Basic principle ,Instrumentation and applications of SEM, TEM and AFM,*

REFERENCES:

- Instrumental Methods of Analysis*, Willard, Merritt, Dean and Settle, CBS Publisher and Distributors.,**1986**.
- Thermal Analysis*, W. W. Wendlandt and L. W. Collins, Dowden Hutechin and Ross.
- Basic Concepts of Analytical Chemistry*, S. M. Khopkar , Wiley Eastern
- Thermal Methods of Analysis*, Principles, Application and Problems, J. Haines, Blackie Academic and Professional, **1994**.
- Chromatographic Methods*, A. Braithwaite and F. J. Smith, 5th edn. Blackie Academic and Professional, London, **1996**.
- Principles of Instrumental Analysis*, Skoog, Holder, Nieman, Fifth edition Thomson Books ,**1998**.

Prepared By: Dr. N C Kothiyal
Ratified By: Dr. B S Kaith

- 1. Ultraviolet and Visible Spectroscopy :** Various electronic transitions (185-800 nm), Beer- Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.
- 2. Infrared Spectroscopy :** Instrumentation and sample handling. Characteristic Vibrational frequencies of alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of Vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on Vibrational frequencies, overtones, combination bands and Fermi resonance. FT-IR.
- 3. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) :** Definition, deduction of absolute configuration, octant rule for ketones.
- 4. Nuclear Magnetic Resonance Spectroscopy :** General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus cruve-variation of coupling constant with dihedral angle. Simplification of complex spectra-nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei-F,P.
- 5. Carbon-13 NMR Spectroscopy :** General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.
- 6. Mass Spectroscopy :** Introduction, Ion production & detection – EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectroscopy. Examples of mass spectral fragmentation of organic compounds with respect of their structure determination, MALDI, APCI & GSI.

REFERENCES:

1. *Fundamental of Molecular Spectroscopy*, C. N. Banewell, 4th Edition, Tata Mc Graw-Hill Publication, **1995**.
2. *Introduction to Molecular Spectroscopy*, G. N. Barrow, Mc Graw Hill Publications, **1980**.
3. *Spectroscopic Methods in Organic Chemistry*, D. H. Williams and I. Flemings, Tata Mc Graw-Hill Publication, **1994**.
4. *Physical Method in Chemistry*, R. S. Drago, Sunders, **1985**.

Prepared By: Dr. Rajeev Jindal
Ratified By : Dr. B. S. Kaith

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CY-781

Chemistry of Materials

1. Multiphase Materials :

Ferrous alloys , Fe-C phase transformations in ferrous alloys , stainless steels, non-ferrous alloys , properties of ferrous and non-ferrous alloys and their applications.

2. Glasses , Ceramics and Composites :

Glasses : Introduction , manufacturing , types and applications.
 Ceramics and refractories : Introduction , classification , characteristics , properties , some important high refractory materials and their applications.
 Composites : Introduction , constituents , classification , some industrially Important composites , failure modes and applications.

3. Nanomaterials :

Introduction , carbon nanotubes – their synthesis , properties and applications. Nanotechnology in diagnostic applications . Semiconductor quantum dots – synthesis , electronic structure and correlation of properties with size and their applications.

4. Liquid Crystals :

Introduction , classification , chemical constitution and liquid crystalline behavior , molecular ordering in different mesophases , identification of liquid crystals , polymeric liquid crystals , applications of liquid crystals in displays and in thermography.

5. Polymeric materials :

Molecular shape, structure and configuration , crystallinity , stress-strain behaviour, Thermal behaviour , polymer types and their applications , conducting and ferro- electric polymers.

6. Superconductors :

Introduction , types , properties , preparations , structure of superconductors and applications of low temperature and high temperature superconductivity.

7. Fullerenes :

Introduction , synthesis and purification , conductivity and superconductivity In doped fullerenes , chemistry of fullerenes . Properties – optical properties , ferromagnetism and some unusual properties of fullerenes.

REFERENCES:

1. *Solid State Physics*, N. W. Ashcroft and N. D. Mermin, Saunders College Ed. **1976**.
2. *Principles of the Solid State*, H.V. Keer, New Age International Publishers, Ed. **1993**.
3. *Materials Science*, J.C. Anderson and K.D. Leaver, ELBS, Ed. **1971**.
4. *Handbook of Liquid Crystals*, H. Kelker, R. Hatz and C. Schumann, Chemie Verlag, Ed. **1980**.
5. *Solid State Physics*, J. S. Blakemore, Cambridge University Press, **1985**.
6. *Introduction to Material Science and Engineering*, Y. W. Chung, CRC Press, Ed. **2007**.

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Macromolecular Chemistry

- 1. Basics:** Basic concepts: Monomers, repeat units, functionality, degree of polymerization, classification, types of polymerizations, different types of initiators, polymerization in homogeneous and heterogeneous systems and importance of polymers.
- 2. Polymer Characterization:** Polydispersion: Average molecular weight concept - number, weight and viscosity average molecular weights. Measurement of molecular weights - viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers - chemical analysis of polymers, spectroscopic methods, X- ray diffraction studies, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and atomic force microscopy (AFM). Thermal analysis and physical properties of polymers – TGA/DTA/DTG, tensile strength. Fatigue, impact resistance, wear resistance, hardness and abrasion resistance.
- 3. Structure and Properties:** Morphology and order in crystalline polymers - configurations of polymer chains, crystal structures of polymers, morphology of crystalline polymers, strain – induced morphology, crystallization and melting, polymer structure-property relationship and polymer degradation.
- 4. Polymer Processing:** Introduction to plastics, elastomers and fibers. Constituents of plastics – binders, fillers, dyes and pigments, plasticizers, lubricants and catalysts. Fabrication of plastic articles – casting, blowing, extrusion, lamination and moulding: cold moulding, compression moulding, injection moulding and transfer moulding.
- 5. Properties of Commercial Polymers :** Polyethylene, Polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers - Fire retarding polymers and electrically conducting polymers. Biomedical polymers - contact lens, dental polymers, artificial heart, kidneys, skin and blood cells.

REFERENCES:

1. *Textbook of Polymer Science*, F.W. Billmeyer Jr, Wiley, Ed. **2008**.
2. *Polymer Science*, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern, Ed. **2008**.
3. *Contemporary Polymer Chemistry*, H.R. Allcock and F.W. Lampe, Prentice Hall. Ed. **1981**.
4. *Advanced Polymer Chemistry*, Manas Chanda, Marcel Dekker, Ed. **2000**.
5. *Advances in Polymer Science*, H.J. Cantone, Springer, Ed. **1965**.
6. *Polymer Science and Technology*. P. Ghosh, Tata- Mc GRAW HILL Ed. **2004**.

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