DEPARTMENT OF CHEMISTRY

CURRICULUM AND SYLLABI
B. Tech, M. Sc. & Ph D
(CHEMISTRY)

Dr B R AMBEDKAR NATIONAL INSTITUTE OF TECHNOLOGY
JALANDHAR-144 011 (PUNJAB) INDIA
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SCHEME AND SCHEDULE OF COURSES

B Tech 1st Year (Chemistry)

Course Code	Course Title	Hours /week			
		L	T	P	Credits
CYCI-101	Applied Chemistry –A (ME, CE, IPE, CH, TT)	3	1	0	04
CYCI-102	Applied Chemistry –B (CSE, ECE, ICE, IT, EE, BT)	3	1	0	04
CYCI-103	Applied Chemistry Laboratory	0	0	2	02
CYCI-104	Environmental Studies	3	0	0	03

New Scheme-2019

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-501	Stereochemistry and Reaction Mechanism	3	1	0	4
CY-503	Thermodynamics and Chemical Kinetics	3	1	0	4
CY-505	Main Group Chemistry	3	1	0	4
CY-507	Intellectual Properties Rights	3	0	0	3
CY-509 MA-551	Basic Biological Chemistry / Mathematics for Chemists_	3	0	0	3
CY-601	Seminar I	0	0	0	0
CY-511	Organic Chemistry Lab	0	0	8	4
					Total = 22 Credits

SEMESTER II

Course Code	Course Title	Hours /week			Credits
		L	T	P	
CY-502	Quantum Chemistry	3	1	0	4
CY-504	Pharmaceutical Chemistry	3	0	0	3
CY-506	Surface Chemistry, Adsorption and Catalysis	3	1	0	4
CY-508	Principles of Organic Synthesis	3	1	0	4
CY-510	Symmetry and Group Theory	3	0	0	3
CY-512	Molecular Spectroscopy	3	0	0	3
CY-514	Physical Chemistry Lab	0	0	8	4
					Total = 25 Credits

CY-516	Summer Training in Research Lab/Industry (after second semester)	0	0	0	1

SEMESTER III

Course Code	Course Title	Hours /week			Credits
		L	T	P	
CY-515	Chemistry of Transition and Inner-transition Elements	3	1	0	4
CY-517	Physical Methods of Structure Elucidation	3	1	0	4
CY-519	Analytical Principles and Instrumental Methods of Analysis	3	1	0	4
CY-521	Frontiers in Organic Chemistry	3	0	0	3
CY-5XX	Elective-I	3	0	0	3
CY-600	Project Phase I	0	0	4	2
CY-513	Inorganic Chemistry Lab	0	0	8	4

Total = 24 Credits

SEMESTER IV

Course Code	Course Title	Hours /week			Credits
		L	T	P	
CY-518	Frontiers in Physical Chemistry	3	0	0	3
CY-520	Interdisciplinary Topics in Chemistry	3	0	0	3
CY-5XX	Elective-II	3	0	0	3
CY-5XX	Elective-III	3	0	0	3
CY-600	Project Phase –II	0	0	16	8
CY-601	Seminar II	0	0	0	0
Total = 20 Credits					

TOTAL CREDITS= 22+25+24+20+1=92

Dr. B. R. AMBEDKAR NATIONAL INSTITUTE OF TECHNOLOGY JALANDHAR
DEPARTMENT OF CHEMISTRY
LIST OF ELECTIVE COURSES FOR M. Sc. / Ph D CHEMISTRY STUDENTS

Course Code	Course Title	Hours /week			
		L	T	P	Credits
CY-522	Natural Products	3	0	0	3
CY-523	Ligand Field Theory	3	0	0	3
CY-524	Polymer Chemistry	3	0	0	3
CY-525	Bioinorganic Chemistry	3	0	0	3
CY-526	Advanced Inorganic Chemistry – I	3	0	0	3
CY-527	Advanced Inorganic Chemistry – II	3	0	0	3
CY-528	Solid State Chemistry	3	0	0	3
CY-529	Nanochemistry	3	0	0	3
CY-530	Photochemistry	3	0	0	3
CY-531	Environmental Chemistry	3	0	0	3
CY-532	Statistical Thermodynamics	3	0	0	3
CY-533	Industrial Organic Chemistry	3	0	0	3
CY-534	Leather Chemicals	3	0	0	3
CY-535	Drug Design and Development	3	0	0	3
CY-536	Mechanistic Inorganic Chemistry	3	0	0	3
CY-537	Advanced Organic Chemistry	3	0	0	3

LIST OF OPEN ELECTIVE COURSES FOR B. TECH / M Tech / Ph D STUDENTS

Course Code	Course Title	Hours /week			
		L	T	P	Credits
CYOE-401	Molecular Electronic Devices	3	0	0	3
CYOE-402	Polymer Chemistry	3	0	0	3
CYOE-403	Nanoscience & Nanotechnology	3	0	0	3
CYOE-543	Scientific Documentation and Intellectual Property Rights	3	0	0	3

LIST OF COURSES EXCLUSIVELY FOR Ph D STUDENTS

Course Code	Course Title	Hours /week			
		L	T	P	Credits
CY-538	Green Chemistry	3	1	0	4
CY-539	Principles of Instrumental Methods of Analysis	3	1	0	4
CY-540	Advanced Spectroscopy	3	1	0	4
CY-541	Chemistry of Materials	3	1	0	4
CY-542	Macromolecular Chemistry	3	1	0	4

B.Tech Syllabus

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CYCI – 101 Applied Chemistry-A
Part-A
(Common to all branches)

Course objectives:

CO-1: The students will learn about the Phase Equilibrium and their applications in separation of miscible liquids by distillation the students will get exposure of basic and applications of Distribution Law in solvent extraction

CO-2: This unit will introduce students to the various methods of elucidation of Structure of Organic Molecules by Spectroscopic Methods. This will also cover basics and applications of different spectroscopies. The student will learn about their application in the characterization of crystalline materials by Bragg's equation i.e. x-ray diffraction FESEM and TEM.

CO-3: The objective of this unit is to justify the role of various inorganic materials in the Human body. Here the role of various metals in the human body will also be explained.

CO-4: This unit will be an important section for the students and it will introduce students about basic (generation and characterization) and advanced (Lithography) Nanotechnology.

CO-5: This unit will focus on various types of Fuels and lubricants, their mechanism and applications.

CO-6: This unit will introduce students about the various type of hardness present in the water as well as their treatment methods. Further, it will also explain about the boilers and the problems associated with it.

CO-7: The unit will enable student to understand about various types of Corrosion & Protective Coatings, factors influencing corrosion and topics like Electroplating, Metallic coatings etc.

CO-8: The syllabus will conclude with the introduction about various types of cements and composites materials introduction and their constituents and applications

Course Content:

Unit-I

Phase Equilibria and Distribution law: Phase diagramfor one component system, carbon dioxide system, sulphur system, carbon system; Two component systems: Pb-Ag system, Bi-Cd system, KI-H_2O system, Liquid-liquid equilibrium, Azeotropic mixtures, UCST& LCST:Nernst distribution law, Applications of distribution law,solventextraction. (06 lectures)

Unit-II

Structural elucidation of engineering Materials: Lambert-Beer's Law, Principles and applications of U.Visible Spectroscopy, IR spectroscopy: principles and application to simple molecules, Nuclear Magnetic Resonance Spectroscopy and its applications, MRI, X- Ray Diffraction, Electron microscopy (SEM& TEM). (10 lectures)

Unit-III

Biological Inorganic Chemistry: The chemistry of elements in medicine – chelation therapy, Oxygen transport and storage-Myoglobin, Haemoglobin Bohr's effect, Cancer treatment, Anti-arthritis drugs, contributions of individual elements to biological systems. (03 lectures)

Unit-IV

Nano-Science & Technology: Introduction and Classification based on dimensionality: Quantum Dots, Wells and Wires; Carbon Nanotubes, Fabrication of nanomaterials by Physical & Chemical methods; Lithography: Introduction, types of lithography: Applications of nanomaterialas.
(04 lectures)

Part-B
(For ME, CE, IPE, CH & TT)

Unit-I

Fuels & Lubricants: Classification of various types of fuels, Calorific values, Comparison between solid, liquid and gaseous fuels, Caloricfic value of gaseous fuel, Bomb calorimeter, Calculation of calorific value of a fuel byBomb calorimeter, Lubricantsand its function, classification of lubricants, Mechanism of lubrication, Greases or Semi-Solid lubricants, Lubricating emulsions, Properties of lubricating oils, greases, Cutting fluids, Selectionoflubricants. (05 lectures)

Unit-VI

Water treatment: Introduction, Hardness of water, Alkalinity,Determination of hardness by EDTA method; Disadvantages of hard water, Boiler problems: Scale and Sludge formation in boilers, Caustic Embrittlement, Boiler corrosion, Priming and foaming;Water softening methods (internal & external). (05 lectures)

Unit-VII

Corrosion &Protective Coatings: Introduction about various types of corrosions, mechanism of corrosion, passivity, factors influencing corrosion, Metallic coatings:Inorganic coatings (Chemical dip, Anodised oxide, porcelain), Organic coatings(Paints, Varnishes, Enamels, Special paints); Electroplating, Some othermetalliccoatings, (04 lectures)

Unit-VIII

Cement and Composites: Introduction, manufacturing process, Chemical composition of Portland cement, Plaster of Paris, special cements: concrete and RCC; classification of composities, constitments ofcomposities. (05 lectures)

Course outcomes:

CO-1: The students will be able to understand various phenomenon in Phase Equilibrium and their applications in separation of miscible liquids by distillation and Azeotropic Mixtures further the students will get exposure of basic and applications of Distribution Law in solvent extraction

CO-2: This unit will get exposure of spectroscopic Methods used to characterize engineered materials. The student will learn about the application in the characterization of crystalline materials by Bragg's equation i.e. x-ray diffraction FESEM and TEM.

CO-3: The students will be able to understand the role of various inorganic metals in the biological system.

CO-4: This unit will explain the students about synthesis and characterization of nanomaterial's through various methods. It will also provide information about new technology like lithography etc.

CO-5: The students will able to understand about various types of Fuels and lubricants, their mechanism and applications.

CO-6: This unit will learn students about the various type of hardness present in the water as well as their treatment methods through traditional as well as recent methods.

CO-7: The unit will enable student to understand about various types of Corrosion & Protective Coatings, factors influencing corrosion and topics like Electroplating, Metallic coatings etc.

CO-8: The students will get exposure about various types of cements and composites materials introduction and their constituents and applications

Recommended Books:

1. Atkins, P.W., Physical Chemistry, 8th Ed., Oxford University Press,2006

2. P. Ghosh, Polymer Science and technology (2nd Edition),, Tata McGRAWHill,2008.

3. Carraher, Jr C.E. "Introduction to Polymer Chemistry" 3rd Edition CRC Press, Taylor & Francis group.,2012
4. P. Y Bruice, An Introduction to the Study of Organic Chemistry Pearson publications ,2014

5. John R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds (4th edition), Prentice Hall of India Pvt. Ltd.,1978.
6. C. P. Poole Jr. ,F. J. Owens, Introduction to Nanotechnology , Wiley Interscience,2003.

7. L. E. Foster, Nanotechnology Science, Innovation and Opportunity,, Pearson Education,2007.

8. Williams & Fleming, Spectroscopic methods in organic chemistry (4th Edition),, Tata McGRAW Hill,2003.
9. A Text Book of Engineering Chemistry, Shashi Chawla, Dhanpat Rai & Co, 2004.

10. Mallick, A., " Engineering Chemistry", Viva Books Pvt.Ltd.

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CYCI – 102 Applied Chemistry-B
Part-A
(Common to all branches)

Course objectives:

CO-1: The students will learn about the Phase Equilibrium and their applications in separation of miscible liquids by distillation the students will get exposure of basic and applications of Distribution Law in solvent extraction

CO-2: This unit will introduce students to the various methods of elucidation of Structure of Organic Molecules by Spectroscopic Methods. This will also cover basics and applications of different spectroscopies. The student will learn about the their application in the characterization of crystalline materials by Bragg's equation i.e. x-ray diffraction FESEM and TEM.

CO-3: The objective of this unit is to justify the role of various inorganic materials in the Human body. Here the role of various metals in the human body will also be explained.

CO-4: This unit will be an important section for the students and it will introduce students about basic (generation and characterization) and advanced (Lithography) Nanotechnology.

CO-5: This unit will focus on various types of polymer liquid crystals, their introduction, method of preparation and applications.

CO-6: This unit will introduce students about the various types of Conducting Polymers, their types, preparation and their applications in different fields

CO-7: The unit will enable student to understand about various types of Semi-conductors, insulators and Superconductors

CO-8: The syllabus will conclude with the introduction and application of Materials in energy sector and sensor, their introduction and applications.

Course Content:

Unit-I

Phase Equilibria andDistribution law: Phase diagramfor one component system, carbon dioxide system, sulphur system, carbon system; Two component systems: Pb-Ag system, Bi-Cd system, KI-H_2O system, Liquid-liquid equilibrium, Azeotropic mixtures, UCST& LCST:Nernst distribution law, Applications of distribution law,solventextraction. (06 lectures)

Unit-II

Structural elucidation of engineering Materials: Lambert-Beer's Law, Principles and applications of U.Visible Spectroscopy, IR spectroscopy: principles and application to simple molecules, Nuclear Magnetic Resonance Spectroscopy and its applications, MRI, X- Ray Diffraction, Electron microscopy (SEM&TEM). (10 lectures)

Unit-III

Biological Inorganic Chemistry: The chemistry of elements in medicine – chelation therapy, Oxygen transport and storage-Myoglobin, Haemoglobin Bohr's effect, Cancer treatment, Anti-arthritis drugs, contributions of individual elements tobiologicalsystems (03 lectures)

Unit-IV

Nano-Science & Technology: Introduction and Classification based on dimensionality: QuantumDots, Wells and Wires; Carbon Nanotubes, Fabrication of nanomaterials by Physical & Chemical methods; Lithography: Introduction, types of lithography: Applicationsofnanomaterialas. (04lectures)

Part-B
(For CSE, ECE, ICE, IT, EE & BT)

Unit-V

Polymer Liquid Crystals: Introduction, Classifications, Liquid crystalline phases, Chemical constitutions, Identification of liquid crystals, Liquid crystal behavior, Liquid crystalline polymers, Applications of liquid Crystals in Displays. (05 lectures)

Unit-VI

Conducting polymers: Conducting polymers, classification, Conduction mechanism, Synthesis of conductive polymers:Polyacetylene, Poly (*p*- phenlylene), Polyaniline, Poly (Phenylenesulphide), Poly (1,6-heptadiyne), ApplicationsofCPs, (04 lectures)

Unit-VII

Semi conductors, insulators and Superconductors: Semi conductivity in non elemental materials , Preparations of semiconductors, Chalcogen photoconductors , photocopying process Introduction to Superconductors, types of Superconductors, Properties of superconductors , Applications of Superconductors, Electrical insulatorsor Dielectrics. (05lectures)

Unit-VIII

Materials for energy sector &Sensors: Solar cell, Fuel cell, Examples of Fuel Cells, Advantages and limitations of Fuel Cells, Battery, Types of Batteries, Lead Acid Storage cell, Sensors, Actuators, Biosensors: Introductionandapplications. (05 lectures)

Course outcomes:

CO-1: The students will be able to understand various phenomenon in Phase Equilibrium and their applications in separation of miscible liquids by distillation and Azeotropic Mixturesfurther the students will get exposure of basic and applications of Distribution Law in solvent extraction

CO-2: This unit will get exposure ofspectroscopic Methods used to characterize engineered materials. The student will learn about the application in the characterization of crystalline materials by Bragg's equation i.e. x-ray diffraction FESEM and TEM.

CO-3: The students will be able to understand the role of various inorganic metals in the biological system.

CO-4: This unit will explain the students about synthesis and characterization of nanomaterial's through various methods.It will also provide information about new technology like lithography etc.

CO-5: This unit will learn students about the various type of polymer liquid crystals, their formation and application in recent era

CO-5: The students will able to understand aboutvarious types of conducting polymers, their mechanism of formation and their applications

CO-7: The unit will enable student to understand about various types of Semi conductivity in non-elemental materials, Preparations of semiconductors, photocopying process, Introduction,types, properties,applications of Superconductors

CO-8: The students will get exposure about various types materials used in energy sectors such as fuel cell etc. This unit also enriches students about various types of sensor materials and their mechanism.

Recommended Books:

1. *Atkins, P.W., Physical Chemistry, 8th Ed., Oxford University Press,2006*
2. *P. Ghosh, Polymer Science and technology (2nd Edition),, Tata McGRAWHill,2008.*
3. *Carraher, Jr C.E. "Introduction to Polymer Chemistry" 3rd Edition CRC Press, Taylor & Francis group.,2012*
4. *P. Y Bruice, An Introduction to the Study of Organic Chemistry Pearson publications ,2014*
5. *John R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds (4th edition), Prentice Hall of India Pvt. Ltd.,1978.*
6. *C. P. Poole Jr. ,F. J. Owens, Introduction to Nanotechnology , Wiley Interscience,2003.*
7. *L. E. Foster, Nanotechnology Science, Innovation and Opportunity,, Pearson Education,2007.*
8. *Williams & Fleming, Spectroscopic methods in organic chemistry (4th Edition),, Tata McGRAW Hill,2003.*
9. *A Text Book of Engineering Chemistry, Shashi Chawla, Dhanpat Rai & Co, 2004.*
10. *Mallick, A., "Engineering Chemistry", Viva Books Pvt.Ltd.*

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CYCI-103 Applied Chemistry Laboratory

1) Preparation of Urea-formaldehyde resins.
2) Determine the viscosity of test liquids with the help of Ostwald viscometer.
3) Find out the R_f value of the given amino acid by thin layer chromatography (TLC) and identify the amino acid present in a given mixture by TLC
4) Isolation of caffeine from Tea leaves.
5) To determine the molecular weight of an organic compound by depression in freezing point (Rast Camphor method).
6) Find out the ion–exchange capacity of a cation exchanger (Dowex -50).
7) To prepare phenol formaldehyde resin (Bakelite).
8) To determine the ion-exchange capacity of a given anion exchange resin.
9) To synthesize Paracetamol and determine the percentage yield of the product.
10) Determine the equivalent weight of a given acid.
11) Determination of total (temporary and permanent) hardness in water sample using EDTA as standard solution (Complexometric Titration).
12) Separation of Metal ions by paper chromatography.
13) To estimate the nickel content in the given sample using dimethyl glyoxime.
14) To determine the strength of given acid using pH titrations.
15) To determine the strength of given acid using conductometric titrations.
16) To determine the average molecular weight of a polymer.
17) Determine the surface concentration of 1-butanol in aqueous solution.
18) Determine the amount of sodium carbonate and sodium hydroxide in a mixture by titration.
19) Determination of ferrous ions using potassium dichromate by internal indicator.
20) To Purify Common organic solvents by distillation.
21) To Determine the Acid Value of Fat.
22) To prepare the pure sample of phthalimide.
23) Isolation of Casein Protein from Milk.
24) Synthesis of cis- and trans- potassiumdioxalatodiaquochromate (III)
25) Preparation of a conducting polymer.
26) To determine concentration of trace metals by atomic absorption spectrophotometer.

Note: At least 10-12 experiments will be carried out.

Prepared By: Dr Harsh Kumar

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CYCI-104 ENVIRONMENTAL STUDIES

Course Outcomes

CO1 - Understand concepts and methods form ecological and physical sciences and their application in environmental problem solving.

CO2 - Understand the transnational character of environmental problems and ways of addressing them, including interactions across local to global scales and apply systems concepts and methodologies to analyze and understand interactions between social and environmental processes.

CO3-Reflect critically about their roles and identities as citizens, consumers and environmental actors in a complex, interconnected world.

CO4- An interdisciplinary approach to complex environmental problems using basic tools of the natural and social sciences including ecosystems, biology, chemistry, economics, political science and international processes.

CO5- The ability to work effectively as a member of an interdisciplinary team on complex problems involving multiple competing stakeholders and agendas; and it will also help in developing the ability to write effectively about complex environmental problems and do so for both specialist and general audiences with equal facility.

Unit 1: Multidisciplinary nature of environmental studies

Definition, scope and importance (2 lectures)

Need for public awareness.

Unit 2: Natural Resources:

Renewable and non-renewable resources:

Natural resources and associated problems.

a) Forest resources : Use and over-exploitation, deforestation, case studies. Timber extraction, mining, dams and their effects on forest and tribalpeople.

b) Water resources : Use and over-utilization of surface and ground water, floods, drought, conflicts over water, dams-benefits andproblems.

c) Mineral resources : Use and exploitation, environmental effects of extracting and using mineral resources, casestudies.

d) Food resources : World food problems, changes caused by agriculture and overgrazing, effects of modern agriculture, fertilizer-pesticide problems, water logging, salinity, case studies.

e) Energy resources : Growing energy needs, renewable and non renewable energy sources, use of alternate energy sources. Case studies.

f) Land resources : Land as a resource, land degradation, man induced landslides, soil erosion and desertification.

- Role of an individual in conservation of natural resources.
- Equitable use of resources for sustainable lifestyles. (8 lectures)

Unit 3 : Ecosystems

- Concept of anecosystem**.**
- Structure and function of anecosystem.
- Producers, consumers anddecomposers.
- Energy flow in theecosystem.
- Ecological succession.
- Food chains, food webs and ecologicalpyramids.
- Introduction, types, characteristic features, structure and function of the following ecosystem:-

a) Forest ecosystem
b) Grassland ecosystem
c) Desert ecosystem
d) Aquatic ecosystems (ponds, streams, lakes, rivers, oceans,estuaries)

(6 lectures)

Unit 4: Biodiversity and its conservation

- Introduction – Definition: genetic, species and ecosystem diversity.
- Biogeographical classification of India
- Value of biodiversity : consumptive use, productive use, social, ethical, aesthetic and option values
- Biodiversity at global, National and local levels.
- Inida as a mega-diversitynation
- Hot-sports of biodiversity.
- Threats to biodiversity : habitat loss, poaching of wildlife, man-wildlifeconflicts.
- Endangered and endemic species ofIndia
- Conservation of biodiversity : In-situ and Ex-situ conservation of biodiversity.

(8 lectures)

Unit 5 : Environmental Pollution

Definition

- Cause, effects and control measures of:-
  a. Air pollution
  b. Waterpollution
  c. Soil pollution
  d. Marine pollution
  e. Noise pollution
  f. Thermalpollution
  g. Nuclear hazards

- Solid waste Management: Causes, effects and control measures of urban and industrial wastes.
- Role of an individual in prevention of pollution.
- Pollution case studies.
- Diaster management: floods, earthquake, cyclone andlandslides

(8 lectures)

Unit 6 : Social Issues and the Environment

- From Unsustainable to Sustainabledevelopment
- Urban problems related toenergy
- Water conservation, rain water harvesting, watershedmanagement
- Resettlement and rahabilitation of people; its problems and concerns. Case Studies
- Environmental ethics : Issues and possiblesolutions.
- Climate change, global warming, acid rain, ozone layer depletion, nuclear accidents and holocaust. Case Studies.
- Wastelandreclamation.
- Consumerism and wasteproducts.
- Environment ProtectionAct.
- Air (Prevention and Control of Pollution) Act.
- Water (Prevention and control of Pollution)Act
- Wildlife ProtectionAct
- Forest Conservation Act
- Issues involved in enforcement of environmentallegislation.
- Public awareness. (7 lectures)

Unit 7 : Human Population and the Environment

- Population growth, variation amongnations.
- Population explosion – Family WelfareProgramme.
- Environment and humanhealth.
- HumanRights.
- Value Education.
- HIV/AIDS.
- Women and ChildWelfare.
- Role of Information Technology in Environment and humanhealth.
- Case Studies

(6 lectures)

Unit 8: Field work

- Visit to a local area to document environmental assets-river/forest/grassland/hill/mountain
- Visit to a local polluted site-Urban/Rural/Industrial/Agricultural
- Study of common plants, insects,birds.
- Study of simple ecosystems-pond, river, hill slopes, etc. (Field work Equal to 5 lecture hours)

References:

1. Environmental Studies, Benny Joseph, 3rd Addition, McGraw Hill Education (India) Private Limited, 2018.
2. Environmental Studies, Deeksha Dave, S.S. Katewa, Cengage Learning India Pvt. Ltd., 2012.
3. Environmental Chemistry, 7th Addition, A.K. DE, New Age International (P) Limited,2010.
4. Environmental Science, Anubha Kaushik, C.P. Kaushik , New Age International (P) Limited, 2011.
5. Environmental Studies,Reach Bharucha, 2004.

M.Sc Syllabus

SEMESTER – I

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CY-501 Stereochemistry and Reaction Mechanism

Course Objectives:

To provide basic knowledge of reaction intermediates, reaction mechanism, types of reactions and stereo chemistry of organic compounds.

Course Contents:

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 Intermediatates:** Generation, structure and reactions of carbocations, carbanions, nitrenes and freeradicals.
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 andelectrophiles.
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 Grignardreagents.
7. **Elimination Reactions:** Reaction mechanism, Direction, stereochemistry, formation of alkenes , alkynes and other multiplebonds.
8. **Ring Expansion and Contraction:** Demjanov ring expansion, Favorskii rearrangement.

Course Outcomes:

Students learn about basic of reaction mechanism, types of reactions and stereo chemistry of reactions.

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.

Prepared By: Dr Jaspreet Kaur

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CY-503 Thermodynamics and Chemical Kinetics

Course Objectives:

1. To understand the third law of thermodynamics and its applications
2. Thermodynamic properties of fluids and gases, and energy and mass equilibrium.
3. To understand the law of equilibrium and response of equilibria to conditions.
4. To understand the various theories of chemical kinetics based on classical to statistical approach
5. To understand the dynamics of fast reactions.

Course Content:

1. **Law of Thermodynamics:** Exact and Inexact Differentials, Cyclic Rule, Reciprocity Characteristics, Homogenous Function, Euler's Theorm, third Law of thermodynamics, Nernst Heat theorm, Thermodynamic Properties at Absolute Zero, Entropy & Third Law ofThermodynamics.
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 ofMixing.
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.

Course Outcomes:

Students will be able to

1. To calculate thermodynamic properties of components in a mixture,
2. To set up and solve complex phase equilibrium problems,
3. To set up and solve complex chemical equilibrium problems.
4. To calculate the value of the activation energy for a chemical reaction given values for the rate constant at several different temperatures.

5. To use the Collision Model of Chemical Kinetics to describe how changes in concentration or temperature affect rates of chemical reactions.

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, 3rdEdition.
5. *Chemical Kinetics* by K. A. Cornors, 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-505 Main Group Chemistry

Course Objectives:

1. To understand the importance of H-bonding.
2. To know the reactivities of metals and inert pair effect.
3. To impart knowledge about the formation of coordination complexes.
4. To develop an understanding of the tendency of lighter elements to form electron deficient compounds.
5. To view the structural features of silicates and organosilcon compounds.
6. To explain the chemistry of non-metals to form chains, rings and cages.
7. To comprehend the vast chemistry of interhalogens.
8. To be aware of ozone layer and CFC's.
9. To apprehend the compounds of xenon and krypton.
10. To recognize the importance of group 12 elements.

Course Content:

1. **Chemistry of hydrogen and noble gases:** Isotopes and ionized forms of hydrogen, Protonic acids and bases, hydrides, The Hydrogen Bond, its influence on Properties and influence on structure, Strength of hydrogen bonds and theoreticaldescription, some natural elegant examples of H-bonding, Information about H-bonding from various techniques like IR, NMR and X-ray. Noble gases: introduction and oxidation state survey, noble gas clathrates ,haides, oxidesand other compounds : synthesis, reactivity and stereochemistry. **(08 lectures)**

2. **Chemistry of S-block metals:** Introduction and oxidation state survey, standard redox potentials of alkali and alkaline earth metals, lattice energy and hydration energy and diagonal relationship. Structure and synthesis of Hydrides, Halides, Oxides, Peroxides, Superoxides, Suboxides, Hydroxides, Oxoacid salts, compounds with nitrogen and carbon and complexes of s-block elements. Coordination Complexes of Crowns and Crypts of Alkali and Alkaline EarthMetals ions. **(12 lectures)**

3. **Chemistry of group 12 elements:** Introduction, Similarities and differences between these elements and traditional elements, oxidation state, Chemistry of the elements : reactivity ,standard redox potentials, their combination with halides. Chalcogenides and their related compounds, oxygen, sulphur and halogen compounds, Formation of coordination complexes, Low valent compounds. **(5 lectures)**

4. **Chemistry of Boron, Aluminum and Silicon:** Borides, Boranes, Bonding in boranes, topology of boranes, synthesis and reactivity. Wade's rules,Carboranes and metallocarboranes,Borazine and boron nitride. Chemistry of boron and Aluminum Halides, Amphoteric nature of Aluminium oxides. Potash alum and Aluminum Alkyls. Low oxidation state Alcompounds.Organosilicon Compoundslike carbosilanes, stability of disilenesand silicones. **(5 lectures)**

5. **Inorganic chains, rings, Cages, Clusters and Polymers**: catenation, heterocatenation,

intercalation chemistry, Heterochains, one dimensional conductors, Isopolyanions, polymerization of non-metal anions. Rings: Phosophazenes: synthesis and bonding, Cyclophosphazenes, , Polyphosphozenes polymers and their reactivity, other heterocyclic inorganic ring systems of sulphur, synthesis and structure of homocyclic inorganic ring systems,rings of +3 oxidation state, $(RP)_n$ compounds, , cyclic thiophosphoric acid, pentaphosphocyclopentadienides. **(07 lectures)**

Cages : Simplestcage type molecule P_4, phosphorous oxides, structures of P_4cages , chemistry of P and S, Moleccular structures of some phosphorous sulfides, Arsenic sulfides, Nonmetallic inorganic cages : synthesis andstructures,Introduction of metal clusters, dinuclear compounds : Molecular orbital diagram and molecular structures of metal – metal bonding. **(05 lectures)**

6. **Chemistry of halogens:**Interhalogens : Introduction, Diatomic, Tetraatomic, hexa-atomic and octa-atomic interhalogens: Synthesis, physical properties, chemical reactions, fluorinating agent,as ionizing solvent and electrical conductivity, Lewis acid behavior. Polyhalide and polyhalonium ions of diatomic interhalogens, Reactivity sequence of various interhalogens. Structures and bonding in some polyiodide anions,Pseudohalogens, Cholorofluorocarbons. **(10 lectures)**

Course Outcomes:

1. Importance of H-bonding in natural processes is appreciable . Had there been no H-bonding, there would not have been life on earth.
2. Recognition of capability of s-block elements and group 12 elements to form coordination complexes as the latter are having many similarities with the former.
3. Realisation of importance of silicon as it is the second most abundant element on earth's crust after oxygen and it occurs as SiO_2 and silicate materials.
4. Consciousness about environment.
5. Fathom of inorganic chains, rings, clusters and polymers.

References:

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

Prepared By: Dr Sangeeta Obrai **Rectified by: Dr Vimal Kumar**

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CY-507 Intellectual Properties Rights

Course Objectives:

The course aims to improve the understanding of students regarding Intellectual property (IP) rights, its importance, why protection of IP is needed and how their protection and promotion can help our society. Generally, students are aware of IP rights such as copyrights but the deep knowledge about why and how to protect these rights will be cover under this course. Students will learn about various IP rights such as Trademarks, Patents, Geographical Indications, Traditional Knowledge, etc. In addition, this course will provide key information to student about the research related activities including publication, citation, plagiarism, literature survey, etc. that will improve their scientific learning and presentation skills.

Course Content:

SECTION-A

1. **Introduction**: Intellectual property rights, promotion and protection concepts, classification, copyright and trade marks. (**4 Lectures**)
2. **W T O and W I P O**: Structure, functions and mandate. (**3 Lectures**)
3. **Patents**: Difference between discovery and invention. Patentable inventions, rights of patent owners. (**3 Lectures**)
4. **Copy Right and Trade Mark**: Differences, advantages and limitations. (**3 Lectures**)
5. **Geographical Indicators**: Geographical indicators and their protection. Difference between geographical indications and trademark. (**4 Lectures**)
6. **Industrial Design**: Industrial design, protection of industrial design. (**2 Lectures**)
7. **Traditional knowledge**: Scope, limitations and disputes. (**2 Lectures**)
8. **TRIPS Agreement**: Salient features, duration and transitory provisions. (**3 Lectures**)
9. **National and International Registration Systems**: The patent corporation treaty (PCT), main international agreements. (**3 Lectures**)
10. **Indian Patent Rules**: The Patents Act 1970, The Patent Rule 2003 as amended and effective from 1. 1. 2005, salient features. (**3 Lectures**)

SECTION-B

1. **Scientific Documentation and Presentation Skills:** Literature survey, citation of references in the texts,abstract, graphical abstract, keywords, plagiarism, cover letter to Editor, exercises for scientific documentation, scientific presentation skills, group discussions, On-line paper submission, transfer of copyright, Referee's comments, awareness about Citation indices: Impact Factor, Average Impact Factor, Total Impact Factor, Citations, h-index and i10-index, Citescore, SNIP, Open access publications. (**10 Lectures**)

Course Outcomes:

Through this course student will learn:

1. To develop theoretical knowledge and development about IP rights.
2. Why protection and promotion of various intellectual property is needed.
3. How to protect IP rights Nationally and internationally.
4. Legal protection of new creations
5. Dependence of economic growth, creation of new jobs and industries, and enhancement in the quality and enjoyment of life related to IP protection and promotion.
6. How as an author student can publish their work.
7. Scientific presentation skill.
8. How to file a patent in India
9. What are the various disputes raised in India due to negligence in protecting IP.

References:

1. D. Vaver, Copyright Law, Irwin Law Incorp., Toronto, ISBN 1-55221-034-0, 2000.

2. Drahos , Peter, Adlershot Intellectual Property, Darmouth, ISBN 1840147407, 1999.

3. Cornish, William R, Intellectual Property: Patents, Copyright, Trademarks and Allied rights London: Sweet and Maxwell, 4th Edition , ISBN: 0421635401, 1999.

4. World Intellectual Property Organization, Intellectual Property Reading Material, 2nd Edition, ISBN: 92-805-0756-7, 1998.

5. Ladas, Stephen P, Cambridge, Patents, trademarks and related rights: National and International Protection, MA: Harvard University Press, ISBN: 06746577756, 1975.

6. Universal's The Patent Act (39 of 1970) with amendments-Universal Law publishing 2005.

7. D. I. Brainbridge, Intellectual Property, 8th Edition, Pearson Education Limited, ISBN 978-1-4082-2928-6, 2010.

Website of WTO and WIPO for current and updated materials: DL 001 and DL-101 courses of WIPO

Prepared By: Professor Balbir Singh Kaith **Rectified By: Dr Vickram Jeet Singh**

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CY-509 Basic Biological Chemistry

Course Objectives:

1. To strengthen the idea of students about different types of cells, their structures and functionality.
2. Introducing major biomolecules like carbohydrates, protines, amino acids, lipids and phospholipids to the students with their specific details and to discuss the role of biological membranes in transportation.
3. To provide details about nucleic acids and their role in biological functions.
4. To demonstrate the kinetics and mechanism of reactions involving enzymes.
5. To provide the knowledge about nutritional requirements, cholesterol, diet and weight, nutrition and cancer, interaction between food and drugs.
6. To provide the knowledge about water contamination and its treatment.
7. To provide the knowledge about landfill technologies.

Course Content:

1. **Cell:** Types of cells, structure and functions. **(05 lectures)**
2. **Introduction to Biomolecules:** Carbohydrates, Proteins, Amino acids, Lipids and Phospholipids. **(08 lectures)**
3. **Nucleic Acids:** Base pairing, double helices, DNA replications, transcription and translation. **(06 lectures)**
4. **Enzymes:** Enzyme kinetics and mechanism, nature and application of enzymes. **(04 lectures)**
5. **Body Fluids:** Digestive fluids, blood, hemoglobin and respiratory gases, sickle-cell anemia, blood-clotting, acid-base balance, physiological disorders of acid-base regulation. **(06 lectures)**
6. **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 and biological membranes and transport mechanism. **(12 lectures)**

Course Outcomes:

1. The students will get exposure about the various types of cell organism and their functions.

2. The students will get exposure about the various biomolecules like amino acids, carbohydrates , lipids etc.
3. The students will get idea about the genetic coding and knowledge of DNA and RNA.
4. The students will get exposure about various types of enzymes and their functions.
5. Finally the syllabus will end with the detail information about the various types of body fluids and their actions alongwith the important topic about health, diet and environment**.**

References:

1. Principles of Biochemistry, Lehninger 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. Biokess, Kenneth Breslauer and Edward Edelson, Prentice-Hall, New Jersey, Ed.1986.

Prepared By: Dr B S Kaith **Rectified by: Dr Uma Shanker**

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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 bymatrices.

2. **Vectors:** Scalar and vector quantities, vector addition and law of addition, commutative and associated law, vector multiplication. Vector differential operator Del, Gradient, Divergence andCurl.

3. **Functions:** Real functions, operations on Real functions, Intervals (closed and open) Even and odd functions, periodicfunction.

4. **Limits:** Introduction, Units, Formal Approach to limit, Algebra of limits, Evaluation oflimits.

5. **Continuity:** Continuous function, Continuity in an interval, Properties of continuous function. Domain ofcontinuity.

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 partialfractions.

8. **Differential Equation:** Definition and formation of differential equations, solution of different equations of first order and first degree: variable separable, homogeneous function Leibnitz's linearequations.

REFERENCES:

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

Prepared By: Dr. Geeta Partap
RatifiedBy: Dr. JaspalSingh

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CY-601 Seminar I

(Compulsory for M.Sc 1st year)

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CY- 511 Organic Chemistry Lab

1. **Distillation &separation**
   (a) To purify common organicsolvents
   (b) Extract rose oil from rose petals by steamdistillation.
   (c) Separation of givenmixtures.
2. **Chromatography**
   (a) To separate plant pigments by columnchromatography.
   (b) Identification of phytoconstituents using thin layerchromatography.
   (c) Identification of sugars in fruit juices through paperchromatography.
3. **Organicanalysis**:
   Detection of common functional groups in the given organic compounds and identification of compound through derivatives.
4. **Organicpreparations:**
   1. Cinnamic acid by perkinreaction
   2. Benzaldehyde by Beckmannrearrangement
   3. Chalcone by Aldolcondensation
   4. Ethyl p-aminobenzoate(benzocaine)
   5. Prepration of Benzopinacolone by Pinacol-Pinacolonerearrangement
   6. Synthesis ofN-phenylmaleimide
   7. Preparation of p-bromoaniline fromacetanilide.
   8. Preparation of Phenacetin fromp-aminophenol
   9. Preparation of eosin from phthalicanhydride
   10. Preparation of p-chlorobenzoic acid fromp-toluidine.
5. **Biochemical preparations/Estimations**
   1. Determination of acid value ofoils.
   2. Determination of Saponification value of given oil/fat.
   3. Determination of Iodine number offat.
   4. Isolation of casein frommilk.
   5. Isolation of Caffeine from teaLeaves.
6. **Quantitativeanalysis**
   1. Estimation of glucose in the givensample.
   2. Estimation of number of amino groups inaniline.
7. **Physical methodDetermination**
   The synthesized compounds will be characterized on the basis of ^{1}H, ^{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

SEMESTER – II

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CY-502 Quantum Chemistry

Course Objective:

The primary objective of this course is to develop familiarity with the physical concepts and facility with the mathematical methods of quantum mechanics. A secondary, but still very important objective is to cultivate the skills at formulating and solving the problems. A subsidiary objective is to encourage the development of self-discipline and work habits that are useful both in academic course work and in the real world

Course Content:

1. **Foundations of Quantum Mechanics:** Operators, Postulates, Matrices and SchrodingerEquation. [4 hrs]
2. **Linear Motion and harmonic Oscillators:** Translational, harmonic, particle in a box a penetration throughbarriers. [5 hrs]
3. **Rotational motion and hydrogen atom:** Particle in a ring & on a sphere, motion in a columbicfield. [5 hrs]
4. **Angular momentum:** Angular momentum operators, definition of states, Composite systems. [4 hrs]
5. **Techniques of Approximation:** Perturbation theory, variation theory, HF theoretic, time dependentperturbation. [4 hrs]
6. **Atomic Structure:** Hydrogen, Helium & multi electronsystem. [4 hrs]
7. **Molecular Structure:** Born- openheimer approximation MO theory of mono, dia & polyatomic molecules, band theory ofsolids. [4 hrs]
8. **Electronic Structure:** SCF method electron correlation Density functional theory, gradient method, semi-empirical methods & software packages forcalculations**.** [4 hrs]
9. **Molecular Rotation & Vibration:** Rotation & Vibration in diatomic, polyatomic molecules. [4 hrs]
10. **Electronic Transition in molecules:** Rotational, Vibronic and electronic states & fates of excitedspecies. [4 hrs]

Course Outcomes:

This senior-standing course presents a “Modern Approach to Quantum Mechanics”. This means that it describes the concept of quantum mechanics directly . To say it in other words, the student will experience quantum mechanics as operator theory . In addition the student should realize that quantum mechanics is more than a physical theory, it is a theory of

provocative implications and a great intellectual achievement and adventure.
In particular, the student should:

1. Deal with the formalism of quantum mechanics and associate physical observable with Hermitian Operators.
2. Realize operators can be represented by matrices for which one seeks eigenvalues andeigenvectors.
3. Learn the properties of the Rotation operator, the Hamilton operator as time evolution
4. operator and the momentum operator as translation operator.
5. Comprehend how measurements are interpreted in quantum mechanics.
6. Receive intensive training in the study of quantum systems in different situations: time evolution, solving the Schroedinger equation in one and three dimensions for different potentials.
    a. Understand the basic concept of the time-independent variation and perturbation theory and its application to physical situations.
    b. Follow the basic concept of molecular structure and electronic structure.

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**

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CY-504 Pharmaceutical Chemistry

Course Objectives:

1. To make the students aware about the development and discovery of new drugs.
2. To impart knowledge about the action of drugs on the desired target (receptor) sites.
3. To study different types of drug-target interactions and drug design.
4. To study different pharmacokinetic issues including chemical and metabolic stability.
5. To impart knowledge about prodrugs and their activation by external factors.
6. To describe mode of drug administration including oral, inhalation, injection and implants.
7. To study the different types of phases involved in clinical trials and the final marketing of the drugs.

Course Content:

1. **Drug Discovery and Drug Development:** Introduction, Present and Past, Drugs and the medicinal chemist, Classification of drugs, Drug targets specification, Choice of Bioassay, i*n-vivo and in-vitro* tests, Pitfalls. **(06 lectures)**

2. **Drug Actions 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. **(04 lectures)**

3. **Drug Design, Drug Target Interactions:** Introduction, Variation of substituents, Expansion of the Structure, Chain expansion/ Contractions, Ring expansion/ Contractions, Ring Variation, Ring Fusions, Isosteres. **(06 lectures)**

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. **(08 lectures)**

5. **Prodrugs :** Introduction , Effect of prodrugs on : improved membrane permeability, prolonged drug activity, masking drug toxicity and side effects, increased chemical stability targeting of groups, prodrugs activation by external influence. **(06 lectures)**

6. **Cimetidine:** A rational approach drug design, Introduction, Histamine, searching and developing of lead compound, partial agonist to antagonists, development of metiamide and cimetidine (biological activity structure and activity, metabolism and synthesis). **(06 lectures)**

7. **Drug administration:** Introduction, oral administration, sublingual administration, rectal administration, epithelial administration, inhalation, injection and implants. **(04 lectures)**

Course Outcomes:

1. The students will get exposure about the various types of drugs and their development processes.
2. The students will get exposure about the various types of drugs and receptors and the drug-target interactions.
3. The students will get exposure about the drug design, drug target interactions and Pharmacokinetics.
4. The course will finally provide in depth information to the students about prodrugs and drug administrationand clinical trials.

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 **Rectified By: Dr Uma Shanker**

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CY-506 Surface Chemistry, Adsorption and Catalysis

Course Objectives:

The objectives of this course are to make the students:

1. Familiar with the concepts of surface chemistry.
2. To understand interdisciplinary nature of the subject with its Industrial applications.
3. To understand adsorption as a surface phenomenon, Chemistry of surfactants, sol-gel synthesis and their application in life
4. To understand the role of catalyst on reaction, kinetics
5. To understand principles of modern methods of Synthesis and characterization of nano particles /nano surfaces and their applications.

Course Content:

1. **Introduction to Surface and Chemistry**: Industrial and day to day Applications of Surface & Colloids Chemistry. Surface Tension, surface energy, Temperature dependence of surface tension, Effects of surface tension, Interfacial tension, contact-angle, wettability measurement of Surface and Interfacial Tesnsions, viscosity, temperature dependence of viscosity Reynolds number. **(10 lectures)**

2. **Adsorption:** Adsorption of gases by solids, Adsorption of solids from solution, measurement of adsorption, factorsaffecting adsorption, Adsorption Isotherms, Gibbs adsorption equation, BET Theory. **(5 lectures)**

3. **The colloidal state:** types, classification, size range, preparation, properties, purification (Dialysis, electrodialysis, ultra filtration), general properties, electrical properties, origin of charge on colloidal particle and stability of sols. Electrical concept of double layer, DLVO theory, DLVO forces, Zeta potential, coagulation or flocculation of colloidal solution. The balance of repulsion and attraction, Applications of zeta potential, protective colloids, gold number, coagulation of sols (by electrolytes), Hardy and Sechulze rule, flocculation value, other methods of coagulation (such as Dialysis, Mechanical means etc), kinetics of coagulation. spontaneous ageing of colloids. **(10 lectures)**

4. **Electro kinetic effect**: electro osmosis, electrophoresis/cataphoresis, Streaming potential, dorn effect or sedimentation potential. Determination of size of colloidal particles. **(04 lectures)**

5. **Surfactants:** types, structure properties, association of colloids, CMC, micelles. Micellization, Kraft temperature, structures of micelles, properties. Determination of CMC, emulsion, macro and micro emulsions, factors determing types of emulsions, characteristics of emulation, emulsifying agents, theories of emulsification, application of micro emulsions, GELs, Sol-Gel transformation, thixotrophy. **(06 lectures)**

6. **Catalysis:** Homogenous and Heterogeneous Catalysts, Acid base catalysis, Biocatalysts, Micellar catalysis, Mechanism of few catalyticreactions. **(04 lectures)**

7. **Nanoscience:** Creation, characterization and applications **(02 lectures)**

Course Outcome:

At the end of the course students should be able to:

1. Design process to removal of toxic compounds from industrial wastewater.
2. To understand fundamental of interactions between surfaces of gases, liquids or solutions and how interfaces are important in many technological and biological processes.
3. Explain adsorption process and its mechanisms on the surfaces.
4. Treatment of portable water requirements.
5. How to catalyst alter new path for chemical reactions.
6. Colloids and how to destabilize dispersed phase particles. Sedimentation process ,Zeta potential and its industrial applications
7. Type of emulsion and applications in daily life etc.

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.

Prepared By: Dr. Harsh Kumar **Ratified By: Dr. N C Kothiyal**

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CY-508 Principle of Organic Synthesis

Course Objectives:

1. To impart knowledge of named reactions & various reagents used in organic synthesis for various organic transformations.
2. To get familiar with alternative methods of synthesis using PTC.
3. The energetics kinetics & investigate of reaction mechanism using various techniques.
4. The knowledge of important class of reactions for synthesis of various heterocyclic i.e. pericyclic reactions.

Course Content:

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, investigationmethods.

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 syntheticapplications.

4. **Reagents in Organic Synthesis:** Anhydrous aluminium chloride, aluminium isopropoxide, boron trifluride, 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, $NaBH_4$, Wilkinson'scatalyst.

5. **Name Reactions:** Aldol condensation, Allyllic Rearrangement, Baeyer- Villiger Rearrangement, Beckmann Rearrangement , Brich 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 TiemanReaction.

6. **Pericyclic Reaction:** Introduction, electrocyclic reactions, theoretical explanation, conservation of orbital symmetry, cycloadditon reactions, frontier molecular orbital approach, sigmatropicrearrangements.

7. **Ring closure and opening reactions:** Formation and opening of rings, Diekmann reaction, Baldwin Rules, Robinson-Annelation, Michael-Robinson addition Thorpe Ziegler reaction, Acylation Cycloaddition, Diels-Alder reaction, Simmons-Smithreaction.

Course Outcomes:

1. Students will get familiar with various reactions, reagents mechanism along with application s of these reactions.

2. Students will get familiar with alternative methods of synthesis.
3. Critical study of reaction mechanism their investigation and applications will impart deep insight to students for various organic reaction studies
4. Students will get knowledge about pericyclic reactions and ring formation reactions for synthesis of various heterocyclics.

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. Ahluwaliaand 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. Starkesand C. Liotta, Acedemic Press, Ed. 1998.
7. Crown Compounds Their Characteristics and Applications, M. Iraoka, Amesterdam, Ed.1982.

Prepared By: Dr Jaspreet Kaur

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CY-510 Symmetry and Group Theory

Course Objectives:

1. To educate students about the importance of symmetry elements and operations and the relations among symmetry elements.
2. To acquaint students with character tables.
3. To develop an understanding of applications of symmetry to group theory.
4. To know the application of symmetry and group theory in (a) molecular orbital theory for organic and inorganic molecules separately and (b) ligand field theory with respect to symmetry properties.

Course Content:

1. **Symmetry elements and operations :**Introduction of symmetry, symmetry operations and symmetry elements : Symmetry planes and Reflections, Inversion centre, Proper axes and Proper rotations, Improper axes and Improperrotations. **(05 Lectures)**

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, classes of symmetry operations, similarity transformations, symmetry classification of molecules with illustrative examples, linear molecules, symmetries with multiple high order axes of five platonic solids. **(07 Lectures)**

3. **Representations of groups :**Important rules about irreducible representations and their characters with illustrations, Relationship between reducible and irreducible representations with examples, Areas of charactertables , construction of charactertables. **(05 Lectures)**

4. **Molecular orbital theory and its applications :**Symmetry based selection rules for cyclisation reactions, Dimerization of ethylene, correlation diagrams for electronic states, Diels-Alderreactions. **(05 Lectures)**

5. **Molecular orbital theory for inorganic compounds :**Transformation properties of atomic orbitals, Angular wave functions, Molecular orbitals for sigma bonding in tetrahedral and octahedralmolecules, SALCs. **(05 Lectures)**

6. **Ligand Field theory :**Introductory remarks, Electronic structure of free atoms and ions, Quantum numbers for many electron atoms, different cases of d^2 electron configurationlevels andterms in a chemical environment, Russell Saunders coupling , *jj*coupling and spin –orbital coupling, coupling schemes: splitting ofcomplete spectroscopic terms. **(06 lectures)**

   Term symbols for p^2 and d^2 electronic configurations Haund's rule, calculation of no. of microstates, selection rules,Splitting of terms of free ions into Mulliken symbols in tetrahedral and octahedral fields, construction of

energy leveldiagram.Special features of electronic spectra of some complexes, Tanabe –Suganodiagrams,Splitting of one electron levels in an octahedral environment, construction of energy leveldiagram.

(07 lectures)

Course Outcomes:

1. Students acquire full knowledge of symmetry elements and operations and the relations among symmetry elements.
2. Students come to know fully about character table and the rules for construction of character table.
3. They understand the purpose of their curriculum while applying application of symmetry and group theory to (a)molecular orbital theory to organic and inorganic molecules separately and (b)ligand field theory with respect to symmetry properties.

References:

1. Chemical Applications of Group Theory, F. A. Cotton, Wiley, 3rd edition,**2004.**
2. Valence Theory, J.N. Murellet. 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.**
5. http:// Vlab.co.in/ba_labs_all.php?id=9
6. Chemistry learning mode Chitrathomas@gmail.com

Prepared by: Dr Sangeeta Obrai **Rectified by:Dr Vimal Kumar**

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CY-512 Molecular Spectroscopy

Course Objectives:

1. The course aims to provide a thorough discussion on the basic principles and applications of modern analytical spectroscopy at the advanced level. Emphasis will be put on the characteristics, analytical aspects, merits and limitations, as well as the practical applications of different spectrochemical methods.
2. Molecular Spectroscopy course provides an introduction to the knowledge of the spectroscopy methods about structure of the chemistry compounds, as well as experimental usage of chosen methods (XRD, ESR, RAMAN and NQR) during the labs.

Course Content:

1. Photoelectron Spectroscopy

Basic principles, photo-electric effect, ionization process, Koopman's theorem.Photoelectron spectra of simplse molecules, ESCA, chemical information from ESCA.Auger electron spectroscopy – basic idea. **(10 lectures)**

2. Nuclear Quadrupole Response Spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant.Applications - halogen compounds and transition metals. **(5 lectures)**

3. X-ray Diffraction

Production of X-rays, Solid state symmetry, Bragg's law, Miller indices, Laue method, Bragg method and Debye-Scherrer method of X-ray structural analysis of polycrystalline materials. **(6 lectures)**

4. Electron Spin Resonance Spectroscopy

Basic principles, zero filed splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, measurement techniques, ESR spectra of paramagnetic organic species, transition metal ions and complexes. **(7 lectures)**

5. Mossbauer Spectroscopy

Quadrupole splitting, Recoil energy, Doppler effect and Chemical Shift. Mossbauer spectrum of ^{57}Fe and ^{119}Sn **(6 lectures)**

6. Raman Spectroscopy

Basic Principles, Raman Scattering, Selection rules, polarization of molecules, Mutual exclusion principle, Raman spectra of rigid and non-rigid diatomic molecules **(6 lectures)**

Course Outcomes:

1. Student will know the basic physical chemistry law that govern molecular spectroscopy.
2. Student will know basic information on molecular methods (Raman, XRD, NQR, and EPR).

3. Student will be able to select molecular spectroscopy methods suitable for solving given scientific problem
4. Student will be able to explain whether the molecular vibrations of a tri atomic molecule are Raman active.
5. Student will be able to explain the difference between Stokes and anti-Stokes lines in a Raman spectrum.
6. Student will be able to justify the difference in intensity between Stokes and anti-Stokes lines.
7. Student will be able to draw the Stokes and anti-Stokes lines in a Raman spectrum of a compound when given the energies of the different transitions.
8. Student will be able to describe the use of powdered XRD.
9. Student will be able to calculate the particle size using Scherer equation.
10. Student will be able to calculate miller indices.
11. Student will be able to structural determination of radicals by ESR.

References:

1. Modern Spectroscopy, J.M.Hollas, John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
6. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
7. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M.Orchin, IBH-oxford.
8. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Willey.
9. Introduction to Magnetic Resonance, A Carrington and A.D. Maclachalan, Harper & Row.

Prepared by: Dr Rajeev Jindal **Rectified by: Dr Uma Shanker**

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CY-514 Physical Chemistry Lab

1. Properties of liquids andsolutions.

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

2. ChemicalKinetics

(a) To determine specific rate of acid catalyzed hydrolysis of Ethyl, Acetate at 248.15^{O}K.
(b) To determine the specific rate of the hydrolysis of Ethyl acetate by Sodium Hydroxide at298.15^{O}K.
(c) To study the rate of acid catalyzed iodination of acetone in the presence of excess acid and action at298.15^{O}K.

3 Surface chemistry andcolloids

(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 onIFT.
(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 itsCMC.
(e) To find out coagulant doses with the help of flocculator for differentsamples.
(f) To remove colloidal particles from potablewater.

4. Thermodynamics

(a) To determine heat of neutralization of hydrochloric acid and sodiumhydroxide
(b) To determine the solubility product of Bariumiodate.

5. Thermo AnalyticalMethods

(a) To study thermal decomposition of copper sulfatepentahydrate
(b) To study the precipitation reaction between silver nitrate and sodiumchloride.

6. Spectrophotometry

(a) To verity Beer's law for solution of KMnO4 and to determine concentration of given unknownsolution.
(b) Analysis of electronicspectrumof organiccompounds

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 nmwavelength.

(b) To study photochemical bleaching of dyes(Methlene blue or malachite green usingspectrophotometer

(c) To study photochemical decomposition ofH_2O_2.

8. Polarimetry

(a) To study the inversion of cane sugar, a first order reaction with the help of Polarimeter.

(b) To determine optical rotation of different optically activesubstances.

9. Miscellaneous

(a) To determine the turbidity with the help of turbiditymeter.

(b) To study conductometric titrations of mixture of acid andbase.

(c) To study pH metric titrations of mixture of acid andbase.

REFERENCES:

1. *Practicals in Physical Chemistry*, P. S. Sindhu, MacMilla 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 McGraw

5. *Experimental Physical Chemistry*, G. P. Methewa, Glaredon Press,**1985.**

6. *Experimental Physical Chemistry*, R. C. Das and B. Bahera Tata Mc Graw **1983.**

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

CY-516	**Summer Training in Research Lab/Industry (after second semesyet) (after second semester)**	**0**	**0**	**0**	**1**

Note:Summer Training is compulsory for M. Sc. 2nd yearStudentsDuring Summer Vacations in some other Institutions / Industries like IITs , CSIR Labs , IOCLetc.

SEMESTER – III

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CY-515 Chemistry of Transition and Inner - Transition Elements

Course Objectives:

1. The course aims to help the students to learn the advanced concepts of Inorganic Chemistry and prepare them for advanced research. It is anticipated that students taking this course should have basic and advanced knowledge of inorganic chemistry of transition and inner transition elements at the postgraduate level.
2. The present syllabus has been framed as per the CSIR NET and recent research trends in the subject. We will cover topics relating to functional group transformations as a refresher with emphasis on the mechanistic aspects. The different topics under different units will be covered in order to bring forth the importance of advanced theoretical and practical concepts of transition elements.

Course Content:

1. **Survey of Transition Metal Chemistry** – Electronic configuration, general characteristics, oxidation states, pi-acid ligands, metal clusters and cages, electronic structures of clusters with π -acid ligands, metal-metal bond, Quadruple bonds, relation of clusters to multiple bonds and one dimensional solids. **(08 lectures)**

2. **Comparative Chemistry of First, Second and Third Transition Series:** The comparative chemistry of the elements, compounds and complexes of **Group 3** (Scandium Group) to **Group 12 (**Zinc group) in different oxidation state. The role of elements of first, second and third transition series in organometallics and bioinorganic chemistry. **(08 lectures)**

3. **Lanthanides and Actinides:** Electronic configuration, oxidation states, coordination numbers and stereochemistry, Magnetism and spectra, complexes and organometallic chemistry of lanthanides and Actinides; Preparation of transuranic elements their application in nuclear chemistry. **(08 lectures)**

4. **Inorganic Reaction Mechanisms:** Classification of redox reaction mechanism, outer sphere electron transfer processes, one electron inner sphere and long range electron transfer processes, two electron inner sphere election inner sphere electron-transfer processes. **(08 lectures)**

5. **Transition Metal Catalyzed Reactions:** Organometallic reagents in organic synthesis and in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerization); pi-acid metal complexes, activating of small molecules by coordination. **(08 lectures)**

Course Outcomes:

On successful completion of the course students will be able to:

1. To develop theoretical knowledge of inorganic chemistry, for the professional practice in academics and in research & development.
2. To develop an understanding of the reactivity trends of a range of transition elements and their compounds in the periodic table.

3. To establish an awareness of the role of inorganic chemistry in the chemical sciences.
4. To develop an understanding of the role of the chemist in measurement and problem solving in inorganic chemistry.
5. To provide an understanding of chemical methods employed for problem solving involving inorganic systems.
6. To develop skills in the scientific method of planning, developing, conducting, reviewing and reporting experiments.

References:

1. Inorganic Chemistry. 4rt edition D. F. Shriver and P. W. Atkins, Oxford University, Oxford, 2006.
2. Advanced Inorganic Chemistry by 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, John Wiley & Sons, 2001.
5. Chemistry of elements, N. N. Greenwood Pergamon Press, 2000.
6. Organomettalics, A Concise Introduction, Ch. Elschenbroich and A. Salzer Second Edition, VCH.

Prepared by Dr Vimal Kumar **Rectified by: Dr Sangeeta Obrai**

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CY-517 Physical Method of Structure Elucidation

Course Objectives:

1. The objectives of this course are to: Introduce the theory of the various instruments and the signals produced when analyzing compound.
2. Equip the student with enough information to be able to interpret signals from spectroscopic instruments.

Course Content:

1. **Ultraviolet and Visible Spectroscopy :** Measurement techniques, Beer – Lambert's Law, Intensity of the electronic transition, Franck-Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra, Chromophores , auxochromes, blue shift, red shift, hypo and hyperchromic effect, Transitions in organic molecules, Woodward rules for conjugated dienes, unsaturated carbonyl groups, extended conjugation and aromatic sterically hindered systems.

   (08 lectures)

2. **Infrared spectroscopy :**Instrumentation and sample techniques, Finger print region, spectral features of some classes of organic compounds - alkenes, alkynes, aromatic compounds, carbonyl compounds (ketones, aldehydes, esters,amides, acids, anhydrides,lactones,lactums and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. Application of IR spectroscopy.

   (06 lectures)

3. **Nuclear Magnetic Resonance Spectroscopy :**General introduction ,Natural abundance of 1H, 13C, 19F and 31P nuclei; The spinning nucleus, effect of external magnetic field, processional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, proton exchange, spin-spin coupling- splitting theory, one, two and three bond coupling, virtual, long range and allylic coupling, magnitude of coupling constant; factors affecting the coupling constant, complex spin- spin interaction between two, three, four and five nuclei(first order spectra), Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents), CW and FT NMR, Relaxation processes, Applications of NMR in structural elucidation of simple and complex compounds.

   (10 lectures)

4. **Carbon-13 NMR Spectroscopy:** General consideration, Chemical shift,NOE and origin of nuclear Overhauser effect. Proton decoupling, Structural applications of 13C-NMR., pulse sequences, pulse widths, spins and magnetization vectors, DEPT, INEPT, Introduction to 2D-NMR, COSY, NOESY, HSQC spectra. **(06 lectures)**

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

molecular ion peak, index of H deficiency, fragmentation patterns for aliphatic compounds, amines, aldehydes, Ketones, esters, amides, nitriles, carboxylic acids ethers, aromatic compounds etc. **(10 lectures)**

Course Outcomes:

1. A student who has met the objectives of the course will be able to:
2. Demonstrate knowledge of the principles behind the following analytical techniques: MS, IR-, NMR- and UV-spectroscopy
3. Combine and evaluate spectroscopic data obtain from the techniques listed above with respect to determining the structure of a given organic compound.
4. Use the term double bond equivalents.
5. Demonstrate knowledge of the terms used within stereochemistry and isomerism and know which effect these may have on the different types of spectra.
6. Analyze EI-MS and ESI-MS spectra with respect to determination/identification of the molecular mass, constituent formula and analysis of characteristic fragmentation patterns for organic compounds.
7. Analyze IR spectra based on knowledge of characteristic functional group frequencies in relation to the molecular structure.
8. Analyze UV spectra based on knowledge of the different electron transitions and be able to use the different empirical rules to determine the position of the absoption maxima from a given structure.
9. Analyze 1H and 13C NMR spectra.
10. Demonstrate knowledge of the characteristic chemical shifts, homo- and heteronuclear coupling constants and decoupling used in an NMR based structur aldetermination.
11. Calculate 1H and 13C chemical shifts from tables and perform a first order spin-spin coupling-analysis.
12. Use the intensities in 1H and 13C NMR spectra and demonstrate knowledge of which effect the following terms has on these: number of nuclei, NOE, relaxation times and exchange.
13. Demonstrate knowledge as to which influence exchange has on labile protons in 1H NMR.

References:

1. Spectrometric Identification of Organic Compounds, Silverstein, R.M. Bassler, G.C. and Morrill, T.C. Wiley, 1991. 29

2. Organic Spectroscopy, Kemp, W. Macmillan, 1987.

3. Application of Absorption Spectroscopy of Organic Compounds, Dyer, J. R. Prentice Hall, 1965.

4. Spectroscopic Problems in Organic Chemistry, liams, D. H. and Fleming, I. WilMcGraw Hill, 1967.

5. Molecular Spectroscopy, Barrow, G.M. Introduction to McGraw Hill.

6. Fundamentals of Molecular Spectroscopy, Banwell, C.N. McGraw Hill, 1966.

7. Introduction to Spectroscopy, Pavia, D.L., Lampan, G.M. and Kriz, G. S. Hartcourt College Publishers, 2001.

Prepared by: Dr Rajeev Jindal **Rectified by: Dr Uma Shanker**

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CY-631 Analytical Principles and Instrumental Methods of Analysis

Course Objectives:

The objectives of the course is to

1. Develop understanding of a wide range of common Analytical Techniques used for analysis of various substances/materials in chemistry with focus on instrumentation and its working.

2. The course also gives basic inputs to understand the interpretation of their results and advantages and disadvantages of each technique and identification and characterization of the materials.

Course Content:

1. **Data Analysis:** Uncertainties, Errors, calibrations, Mean, Standard Deviation , Least square fit,

2. **Atomic Absorption Spectroscopy:** General principles, instrumental set up and analytical procedures andapplications,

3. **Thermo-Analytical Method:** Theory, instrumental requirements and methodology for thermo gravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC),applications

4. **Chromatographic Methods:** Classification of chromatographic methods according to separation and development procedure, Instrumentation and applications (GC andHPLC)

5. **Electrochemical Techniques:** Conductometry, pH metry, Karl Fischer titration, cyclic voltametry,Polarography

6. **Modern Methods of Surfaces and Crystal Analysis:** SEM, TEM, AFM,XRD.

Course outcome:

1. Student will understand basic principle and function of each part while handling the instruction in future

2. He/she will be able to interpret the result and can understand the outcome of his result and its significance.

3. Student can understand modern technique used in analysis of materials and could use them in future.

References:

1. *Instrumental Methods of Analysis*, Willard, Merritt, Dean and Settle, CBS Publisher andDistributors.,**1986.**

2. *Thermal Analysis*, W. W. Wendlandt and L. W. Collins, Dowden Hutechin and Ross
3. *Basic Concepts of Analytical Chemistry*, S. M. Khopkar , WileyEastern
4. *Thermal Methods of Analysis*, Principles, Application and Problems, J. Haines, Blackie Academic and Professional,**1994.**
5. *Chromatographic Methods*, A. Braithwaite and F. J. Smith, 5^{th} edn. Blackie Academic and Professional, London,**1996.**
6. *Principles of Instrumental Analysis*, Skoog, Holder, Nieman, Fifth edition Thomson Books,**1998.**

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

L T P C
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CY-521 Frontiers in Organic Chemistry

Course Objectives:

1. The objective of this course is to familiarize the students about the concept of asymmetric synthesis, and its applications in organic synthesis.
2. The objective of the course is to make student understand the use of disconnection approach in organic synthesis so that they will be able visualise the synthesis of complex molecules with ease.
3. The use of organometallic reagent in organic synthesis will also be covered to give an emphasis on importance of organometallic reagents in organic synthesis.
4. Another objective is to understand the chemistry Natural Products, their biosynthesis and their significance.

Course Content:

1. **Asymmetric Synthesis:** Chiral auxiliaries, methods of asymmetric induction- substrate, reagent and catalyst controlled reactions. Carbon-carbon bond forming reactions through enolates, enamines and silyl enol ethers. Stereoselective addition to C=O groups (Cram, Cram Chelation and Felkin-Ahn models), determination of enantiomeric and diastereomeric excess; enantio-discrimination. Optical and kinetic Resolution. (**8 Lectures**)

2. **Heterocyclic Chemistry:** Structure, preparation, properties and reactions of compounds containing one heteroatom (O, N, S); furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline. Paal-Knorr, Feist-Benery, Hantzsch, Knorr synthesis, Fisher indole synthesis, Madelung synthesis, Skraup, Friedlander, Pfintzinger, Bischler-Napieralski and Pictet-Spengler synthesis. (**8Lectures**)

3. **Concepts in Organic Synthesis:** Retrosynthetic analysis, strategic disconnections, synthons and synthetic equivalents. Umpolung reactivity – formyl and acyl ion equivalents. Linear and convergent synthesis. (**8 Lectures**)

4. **Protection and deprotection in organic synthesis**: Protection and deprotection of various functional groups: a) alcohols b) 1,2-diols c) amines d) carbonyls e) carboxylic acids. (**4 Lectures**)
5. **Pd and Rh in organic synthesis**: Heck reaction, Suzuki reaction, Sonogashira reaction, Stille coupling, Carbonylation, hydroformylation, decarbonylation reactions. Olefin metathesis using Grubb's catalysts, Buchwald reaction and Pauson-Khand reaction. **(4 Lectures)**

6. **Chemistry of Natural Products:** Chemistry ofTerpenes, steroids and alkaloids. Biogenesis of terpenoids, alkaloids and steroids. (**8 Lectures**)

Course Outcomes:

At the end of the course, the student will be able to

1. Explain the concept of asymmetric synthesis.
2. Understanding the physical methods in analyzing the asymmetricity.
3. Understand the methodological concept of connection disconnection in organic synthesis and significance of protecting groups in synthesis.
4. Emphasize the role of various organometallic complexes and reagents in Organic Synthesis.
5. Understanding the chemistry Natural Products and their significance.
6. Understanding of Umpolung chemistry

References:

1. Asymmetric Synthesis – The Essentials, Mathias Christmaw and Stefan Brase, Wiley, Ed. 2007.

2. Asymmetric Synthesis, Garry Procter, Oxford University Press, Ed. 1976.

3. Heterocyclic Chemistry, Malcoln Sainsbury, RSC Publishing, Ed. 2001.

4. Heterocyclic Chemistry, J. A. Joule and K. Mills, Blackwell Publishing Inc., Ed. 2000.

5. Organic chemistry, Claydon, J., Gleeves, N., Warren, S., Wother, P.; (2001), Oxford University Press, UK.

6. Advanced organic chemistry: Reaction Mechanism, Bruckner, R., (2001), Elsevier, 1st edition.

7. Advanced Organic Chemistry Part A and Part B, Carey, B. F. A., Sundberg R. J., (2007). Springer, 5th edition.

8. Some Modern Methods of Organic Synthesis, Carruthers, W., (2004). Cambridge Uni.Press, 4th edition.

Prepared By:-Dr Rajeev Jindal **Ratified by Dr Virender Singh**

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CY-5XX Elective-I

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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-513 Inorganic Chemistry Lab

INORGANIC PREPARATION

Course Objectives:

1. To comprehend the techniques of synthesis and replace the conventional methods with green preparations.
2. To explain the principles applied in qualitative and quantitative analysis.
3. To learn the theory and importance of analytical chemistry.
4. Analysis of chemicals by using green techniques (Spectrophotometric, electroanalytical techniques, Atomic absorption spectroscopy).
5. To have knowledge of various spectroscopic techniques for structural elucidation of compounds.
6. To maintain the healthy and green environment of the laboratory .

Course Content:

1. **Preparation of Inorganic and Coordination compounds, theirpurification, elemental analyses, M.W determination and elucidation of structures by physicalmethods:**

   (a) Synthesis of Tris(acetylacetonato)manganese(III), $Mn(acac)_3$ and their characterization using magnetic succeptibility balance (MSB) and infrared spectroscopy (IR) (GreenPreparation).
   (b) Synthesis and Characterization of Hexamminechromium (III) nitrate $[Cr(NH_3)_6](NO_3)_3$ using magnetic succeptibility balance (MSB) and infrared spectroscopy IR (Green Preparation).
   (c) Synthesis of Iron(III) acetylacetonate and its characterization using magnetic succeptibility balance (MSB) and infra redspectroscopy (IR).
   (d) Synthesis and characterof nitro- and nitritopentamminecobalt (III)chlorides Usinginfra red spectroscopy(IR).
   (e) Synthesis of hexamminecobalt(III) chloride and pentammineaquocobalt(III)chloride.
   (f) Synthesis of cis- and trans-potassiumdioxalatodiaquochromate(III).
   (g) Aquation of trans-dichlorobis(1,2-diaminoethane)cobalt(III)chloride.
   (h) Synthesis and resolution of tris(ethylenediamine)cobalt(II)ion.
   (i) Synthesis of Hexaamminenickle (II) chloride and estimation of Ni(II) in the complex by gravimetry andvolumetry.
   (j) Synthesis oftris(acetylacetanonato)iron(III).
   (k) Synthesis and reactivity oforganocobaloximes.

2. **Qualitative Ion ExchangeTechnique:**

   (a) Separation of zinc and magnesium on an anion exchanger (b)Separation of chloride and bromide on an anion exchanger (c)Determination of the total cation concentration in water (d)Separation of cadmium and zinc on an anion exchanger.

3. **Complexometric Titrations:**

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

4. **Electro Analytical Techniques-pH metric, Conductometricand Amperometric Titration:** Representative acid-base and redoxtitrations.

5. **Colorimetry and Spectrophotometry:**

(a) Determination of λ_{max} the absorption curve and concentration of asubstance
(b)Simultaneous spectrophotometric determination (chromium andmanganese)
(c)Spectrophotometric determination of pK value of an indicator (d)Determination of copper (II) withEDTA
(e) Determination of iron (III) with EDTA.
(f) To find out the stoichiometry of complexes by Job's method.
(g) Determination of stability constant of metal –ligand complex by spectrophotometric titraions using spectrophotometer.
(h) VirtualLabs.

6. **Atomic Absorption Spectroscopy:**

(a) Determination of cations by AAS
(b) Determination of magnesium and calcium in tapwater (c)Determination of trace elements in contaminatedsoil
(d)Determination of vanadium in lubricating oil, determination of trace lead in a ferrous alloy.

7. **Synthesis of Green Reagents:**

a) Tetrabutylammoniumtribromide (TBATB) and itsapplication
b) Ionic Liquid, 1-methyl-3-pentyl-imidazolium bromide, [pmIm]Br and its application

8. **Inorganic analysis by using green methods:**
9. **Qualitative determination by UV, IR, NMR,ESR:**

Course Outcomes:

1. Students became acquainted with various green inorganic preparations, green reagents and green methods of detection of compounds as is recommended by UGC and is the need of hour.
2. Comprehension of various techniques of titration like complexometric and electroanalytical techniques like pH-metric, conductometric and amperometric titrations.
3. Fathom of Structural elucidation of compounds by using various spectroscopic techniques.
4. Appreciation of healthy and green environment as it improves not only the healthbut the confidence and overall personality of the learner.

References:

1. Chemical Curiosites, 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.
7. http:// dst.gov.in/green-chem.pdf

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

Prepared By: Dr. Sangeeta Obrai **Rectified by: Dr Vimal Kumar**

SEMESTER – IV

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CY- 581 Frontiers in Physical Chemistry

Course Objectives

1) To understand the Nuclear chemistry and its various types along with the different models working behind it.
2) To learn about the calculation of molecular weights of Polymers using different methods and kinetics behind the synthesis of polymers.99999
3) To understand the different types of crystal Structures and applications of studying solid state chemistry.
4) To study various types of cells, electrode potential, calculation of EMF and theories of electrochemistry.
5) To understand all possible configurations of a given system, which satisfy the given boundary conditions such as temperature, volume and number of particles, are equally likely to occur.

1. **Statistical Thermodynamics:**Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems. **(10 lectures)**

2. **Electrochemistry:**Nernst equation, redox systems, electrochemical cells; Debye Huckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations. **(12 lectures)**

3. **Solid State:**Crystal structures; Bragg's law and applications; band structure of solids. **(6 lectures)**

4. **Nuclear Chemistry:**Nuclear reactions, Fission and fusion, radio-analytical techniques and activation analysis. **(7 lectures)**

5. **Polymer Chemistry:** Molar masses, Kinetics of polymerization. **(6 lectures)**

Course Outcomes:

After studying the course, the student will be able to:

1. Explain the macroscopic observables associated with nuclear change, Identify and define various types of nuclear transmutation including fission, fusion and decay reactions, Recall and properly use Einstein's theory of relativity equation, $E = mc^2$, to calculate the amount of energy released upon a nuclear change, Understand and explain the concept of isotopic stability including the band of stability, Understand the concept of rate of change and half-life in the context of nuclear decay and Understand the basics of nuclear chemistry applications: nuclear power, medical treatment, isotopic labeling, and carbon dating.
2. Understand the different mechanisms of polymer growth, different methods of calculation of molecular weight of polymers using viscometry, osmotic pressure and Light scattering method
3. Describe the principles concerning solid state structures, use powder diffraction data for characterizing cubic substances, relate diffraction intensities mathematically to structural parameters and derive extinction conditions and electronic properties of solids

4. Apply standard reduction potential data to determine the relative strength of oxidizing/reducing agents, Apply standard reduction potential data to calculate the standard cell potential for an electrochemical cell and from the sign of the potential predict if the cell is voltaic or electrolytic, Calculate the cell potential for a nonstandard cell, Explain thermodynamically the operation of a concentration cell, and be able to predict the concentration in the cell based on the cell potential.
5. Explain the basic concepts and principles in statistical thermodynamics, Use lattice models to study basic phenomena in chemistry and nanoscience, Construct new models based on the basic principles in statistical thermodynamics and Students will learn to recognize, define, and solve problems in equilibrium thermodynamics and statistical physics.

References:

1. Concepts and Model of Inorganic Chemistry, B. Douglas, John Wiley & Sons, 3rd Ed. 2001.
2. Inorganic Chemistry, D. F. Shriver and P. W. Atkins, Oxford University, 4th Ed. 2006.
3. Inorganic Chemistry, J. E. Huheey, Pearson, 4th Ed. 2005.
4. Organic Synthesis - The Disconnection Approach, S.Warren, Willey Interscience, Ed. 1982.
5. Physical Chemistry, P. Atkins and J. D. Paula, Oxford, Ed. 2007.
6. Thermodynamics, Statistical Thermodynamics, and Kinetics, T. Engel and P. Reid, Prentice Hall, Ed. 2006.

Prepared By:- Dr. Rajeev Jindal

L T P C
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CY-664 Interdisciplinary Topics in Chemistry

Course Objectives:

- The main objective of this course is to introduce students about the recent advancement in the interdisciplinary topics such as green chemistry, nanoscience nanotechnology, catalysis and Supramolecular chemistry
- The students will be demonstrated well-developed problem solving skills, applying their knowledge and using their ability to think analytically and creatively about various phenomenon involved in these topics
- Expose both student groups to the social, economic, and ethical issues of these interdisciplinary topics

Course Content:

1. **Nanoscience & Nanotechnology:-** Introduction of nanoscience and nanotechnology, Methods of generation of Nanomaterials, Methods of characterization of nanomaterials, Electron Microscope, XRD, Spectroscopic techniques, Properties and applications of Nanomaterials.

2. **Green Chemistry:-** Introduction, the need of green chemistry, principles of green chemistry, sustainability, atom economy, E-factor, Role of catalyst, solvent, planning of green synthesis, tools of green chemistry, Green reactions, Aldol condensation, Cannizaro reaction and Grignard reaction- comparison of the above with classical reactions- Green preparations, enzymes and other alternate methods of synthesis in green chemistry.

3. **Environmental Science:-** Composition of atmosphere, Chemical and photochemical reactions in the atmosphere, Ozone chemistry, Greenhouse effect, Global Warming, Types of pollution their monitoring and control.

4. **Catalysis:-**Types of catalyst, Reactions, Catalyst synthesis, Catalyst deactivation & regeneration. Various Characterization techniques, industrial catalytic processes, Organometallics in homogenous catalysis.

5. **Supra Molecular Chemistry:** Introduction to supra molecular chemistry, molecular forces, common supra molecules, experimental techniques in supra molecular chemistry, host / guest chemistry, molecular recognition- molecular receptors for different types of molecules including arisonic substrates, supra molecular design strategy & nanotechnology. Supramolecular devices. Supramolecular photochemistry.

Course outcomes:

1. The students will be able to understand the basics as well as advanced topics of Nanotechnology and their applications in current scenario
2. The student learn the importance of green chemistry, role of green chemistry in society and in industry
3. The student will get exposure of advanced topics of Environmental Chemistry and various types of pollutions and their rectification techniques
4. The student will be learning about various types of catalysis and their mechanisms. The student will also get exposure about the various industrial processes that involves catalysis

5. Finally, the students will be able to understand Supramolecular Chemistry and their use in various reactions.

References:

1. Principles of Nanoscience and Nanotechnology, M. A. Shah and Tokker Ahmed, Narosa Publication, Ed. 2011.
2. Nanotechnology Principles and Practices, Sulabha K. Kulkarni, Capital Publication, Ed. 2011.
3. Introduction to Nanotechnology, Charles P. Poole and Frank J. Owens, John Wiley & Sons, Ed. 2003.
4. Green Chemistry: Environment Friendly Alternativs, R Sanghi and M. M. Srivastava, Narosa Publication, Ed. 2009.
5. Green Chemistry: Greener Alternatives to Synthetic Organic Transformations, V. K. Ahluwalia, Narosa Publication, Ed. 2011.
6. Catalysis: Principles and Applications, B. Viswannathan, S. Sivasanker and A. V. Ramaswamy, Narosa Publication, Ed. 2007.
7. Catalysts and Surfaces: Characterisation Techniques, B. Viswannathan S. Kannan and R. C. Dekha, Narosa Publication, Ed. 2010.
8. Environmental Chemistry, B. K. Sharma and H. Kaur, Goel Publishing House, Ed. 1994.
9. Environmental Pollution Analysis, S. M. Khopkar, Wiley Eastern Ltd., Ed. 1995.
10. Supramolecular Chemistry – Fundamentals and Application, Katsuhiko Ariga and Toyoki Kunitake, Springer, 1st Ed. 2006.
11. Green Chemistry, P. T. Anastas and J. C. Warner, Oxford University Press, Ed. 1988.

Prepared By: Dr. Rajeev Jindal/Dr. Jaspreet Kaur Rajput

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CY-5XX	**Elective-II**	**3 0 0 3**
CY-5XX	**Elective-III**	**3 0 0 3**
CY-600	**Project Phase-II**	**0 0 16 8**
CY-601	**Seminar-II**	**0 0 0 0**

ELECTIVES

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CY-522 Natural Products

Course Objectives:

1. The objective of this course is to introduce students about the various natural products present in plants and living organisms.
2. This course starts with the introduction about the Terpenoids which are mainly obtained from the plant kingdom and their structure elucidation of various terpenoids.
3. This course covers with the introduction about the alkaloids which are mainly obtained from the plant kingdom and their structure elucidation of various alkaloids such as nicotine, morphine, cinchonine, quinine etc which are having many medicinal importances.
4. This course also covers information about steroids such as cholesterol and its structure elucidation. Further this course also provides information about a number of vitamins and their structure elucidation.

Course Content:

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 ofterpenoids.

3. **Steroids:** Introduction, Classification, Isolation, Biosynthesis, Structure elucidation, some important types of steroids, Sex hormones (male and female), Adrenal cortisonehormone.

4. **Insects & Plant Growth Regulators:** Introduction, Hormones of endocrine system, Exocrine secretions, Plant growth regulators, Auxins, Gibberellinsetc.

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 VitaminH.

6. **Chemical analysis of phyto-constituents:** Preliminary and confirmatory chemical tests for Alkaloids, Terpenoids, Steroids, Sapogeninsetc.

Course Outcomes:

1. The course provide information about the structure of various natural products present in plants and living organism.
2. The main outcome of the course is to provide experimental evidences based on reaction mechanism in structure elucidation of various natural products such as terpenoids, alkaloids, vitamins, steroids etc.

3. This course provides the properties of many natural products as medicines such as cinchonine, quinine are used as antimalarial activities. There are a number of natural products which are utilizes as drug in the market.

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
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CY-523 Ligand Field Theory

1. **Introduction:** The concept and scope of Ligand Field Theory**,** Crystal Field & Ligand Fields, p & dorbitals. [6 hrs]

2. **Quantitative Basics of Crystal Field:** Octahedral and Tetrahedral Crystal Field Potentials (Voct &Vtet). [6 hrs]

3. **Free Ions in Crystal Fields:** Effect of Cubic Crystal Fields on S,P,D,F,G,H& ITerms. [6 hrs]

4. **Thermodynamic Aspects ofCrystalFields:** CFSE & itsrelationwithlattice energy, Heat of Ligation and Standard ElectrodePotential. [6 hrs]

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 nephelauxeticseries. [6 hrs]

6. **Magnetic Properties:** Magnetic properties of A, E & T Terms, E.S.R and magnetism. [6 hrs]

7. **Non Cubic Symmetry**: Square Planar, Square pyramidal anddodecahedral coordinationcompounds. [6 hrs]

References:

1. *Introduction to Ligand Fields*, B. N. Figis, 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. Figgs & 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**

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CY-524 Polymer Chemistry

Course Objectives:

1. To introduce students about different types of polymers and their applications, as polymers are now essential part of our day by day life in various forms.
2. To teach students about various mechanisms used for the synthesis and characterization of various polymers.
3. To teach students about industrial methods for manufacturing, synthesis, processing of different types of polymers.
4. To teach students about the several applications of polymers which we are utilizing in our day by day life such as in electronics, mechanics, textile etc.
5. To teach students about the advanced industrial applications of polymers such as waste water treatment, drug delivery, biomedical and agriculture.

Course Content:

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 molecularweights.

2. **Polymerization Techniques:** Types of polymerization and their mechanisms i.e. free radical, cationic, anionic and co-ordination polymerization and theirapplications in differentfields.

3. **Molding Techniques:** Introduction, different molding techniques (both for Thermosetting and thermoplastic resins), additives and their functions, applications of different moldingtechniques.

4. **Conducting Polymers:** Introduction, classification, different types of dopings, synthesis, applications in differentfields.

5. **Composites:** Introduction, classification, different types of reinforcing materials and their applications, failure modes, advantages andapplications.

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 toplants.

Course outcomes:

1. By this course students can get information about different types of polymers (Conventional polymers, conducting polymers, composites, biopolymers)
2. By this course students will aware about the behavior of polymers towards various physiochemical conditions. How they are named and how their various properties could be understood experimentally.

3. By this course students will be able to aware about importance, use and application in various fields.
4. By this course students could understand the composition of the polymers as well as their additives which are used to enhance the various properties of polymers.

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

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CY-525 Bioinorganic Chemistry

Course Objectives:

The main goal of the course is to provide basic training in this interdisciplinary area by applying knowledge of coordination chemistry, acid-base, redox, thermodynamics and kinetics in bioinorganic chemistry. It will cover:

1) Role of enzymes in body,
2) Role of metals in biological systems,
3) Metalloenzymes,
4) Metal proteins in electron transfer processes and
5) Role of metal ions in oxygen transport and activation.

Course Content:

1. **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 irreversibleinhibition. **(7 lectures)**
2. **Mechanism of EnzymeAction:** Transition state theory, orientationand steric effect, acid-base catalysis, covalent catalysis, strain or distortion, Examples of some typical enzyme mechanism for chymotrysin, ribonuclease, lysozyme and carboxypeptidaseA. **(5 lectures)**
3. **Metal Ions in BiologicalSystems:**Essential and tracemetals. **(3 lectures)**
4. **Na^+/K^+Pump:** Role of metal ions in biologicalprocesses. **(2 lectures)**
5. **Bioenergetics and ATP Cycle :**DNA polymerization, glucose storage, metal complexes in transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water modelsystem. **(6 lectures)**
6. **Transport and storage ofDioxygen:** Heme proteins and oxygenuptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt andcopper. **(5 lectures)**
7. **Electron Transfer inBiology:** Structure and function of metalloproteins in electron transport processes- cytochromes and ion-sulphur proteins, syntheticmodels. **(6 lectures)**
8. **Nitrogenase :**Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic

and other evidence, other nitrogenases modelsystems. **(6 lectures)**

Course Outcomes:

1. Apply the basic principles in inorganic and general chemistry to interdisciplinary topics in the field of bioinorganic chemistry.
2. Describe the main roles of metal ions in biological processes, and identify the chemical properties that are required to each particular function.
3. Describe the role of metal ions in enzymes involved in acid-base reactions.
4. Describe the role of metal ions that are involved in electron-transfer reactions in biological systems.
5. Describe how oxygen is transported in different species and identify the metal centers involved in this task.
6. Describe the different metal-activation sites in enzymes that are involved in the activation of oxygen.
7. Identify the main toxicological mechanisms of metals and the biological defenses against the toxic effects.

References:

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

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

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CY-526 Advanced Inorganic Chemistry – I

Course Objectives:

1. The course aims to help the students to learn the advanced concepts of Inorganic Chemistry and prepare them for advanced research. It is anticipated that students taking this course should have basic and advanced knowledge of solid state chemistry, electronic spectroscopic concepts of metal complexes, bonding in metal complexes and organometallicchemistry at the postgraduate level.
2. The present syllabus has been framed as per the CSIR NET and recent research trends in the subject. The different topics under different units will be covered in order to bring forth the importance of advanced theoretical and practical concepts of inorganic metal complexes.

Course Content:

1. **Solid-state Chemistry:** Close-packing of Solids, types and structures of Ionic Solids; crystal system and lattices, radius ratio rules; Lattice Energy; Born–Haber Cycles. Structures of AX, AX_2, ABX_3 type compounds, Perovskite Structures, Spinels and Inverse Spinels, Defects in Solids and properties of solids arising out of defect structures, Band theory for metals, insulators and semiconductors. High Tc Superconductors. Applications of Spinels and Perovskite Structures in Superconductors. **(10 lectures)**

2. **Bonding in Transition metal complexes:,** Molecular Orbital, Theory of Complexes-Ligands symmetry orbitals and metal orbitals involved in molecular orbitals formation in octahedral complexes, MOEL diagrams for octahedral, tetrahedral and square planar complexes showing σ and π bonding in transition metal complexes. **(10 lectures)**

3. **Electronic spectra of Transition metal complexes:**

(a) Octahedral and tetrahedral crystal field splittings of d orbitals, CFSE, magnetism and colour of transition metal ions, Jahn-Teller effect and its application; the determination of Dq, β using spectroscopic data including charge transfer spectra; spectrochemical series, nephelauxetic series, magnetism; paramagnetism, ferromagnetism and anti-ferromagnetism.

(b) Spin-spin, orbital-orbital and spin orbital coupling, LS and jj coupling schemes, determination of all the spectroscopic terms of pn , dn ions, determination of the ground state terms for pn , d n , fn ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, two type of electron repulsion parameters, spin orbit coupling parameters (λ) energy separation between different j states. Interpretation of electronic spectra, Orgel diagrams, Tanabe Sugano diagrams. **(10 lectures)**

4. **Organometallic chemistry:** Introduction to Organometallic Chemistry, Synthesis, bonding, structure and reactivity of organometallic compounds. Ideas on M-C bond; Ligands involved, electron count. Bonding in Metal-alkyl, metal-carbonyl, metal-olefin and metal-carbene complexes and metallocenes. Concept of isolobality and stereochemical non-rigidity, Fluxional organo transition metal compounds. **(10 lectures)**

Course Outcomes:

On successful completion of the course students will be able to:

1. To develop theoretical knowledge of various metal complexes, for the professional practice in academics and in research & development.
2. To establish an awareness of the role of inorganic chemistry in the chemical sciences.
3. To develop an understanding of the role of the chemist in measurement and problem solving for different metal complexes.
4. To provide an understanding of electronic spectroscopic methods employed for problem solving in metal complexes.
5. To develop skills in the scientific method of planning, developing, conducting, reviewing and reporting experiments.

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.
6. Organomettalics, A Concise Introduction, Ch. Elschenbroich and A. Salzer, Second Edition, VCH.

Prepared by:Dr Vimal Kumar and Dr Sadhika Khullar Rectified by: Dr Vimal Kumar

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CY-527 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 : lrving William Series. Kinetic aspects : reactions and aquation rates, electron transfer reactions. Reaction mechanism in inorganic reactions. Redoxreactions.
2. **Organometallic Chemistry :**Structure, Bonding and Reactivity studies of metal carbonyls, nitrosyls, dinitrogen complexes, metal alkyls, carbenes, carbines and carbides. Metallocenes and related chemistry. Homogeneous and heterogeneous catalysis. Organometallic complexes with metal-metalbonds.
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 carrierdesign.
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 magneticmaterials.
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 ofnon-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 inPET.

REFERENCES:

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

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

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CY-528 Solid State Chemistry

1. **Electronic structure of solids :**Introduction, Simple non-metallic solids, Transition metal compounds, Defects andimpurities.

2. **Chain compounds and one dimensional physical behaviour :**Introduction. Special features of chain compounds, Structures of chain compounds, Physical properties of chaincompounds.

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 andmagnetism.

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, Multimetalliccatalysts.

5. **Zeolite :**Introduction, Structures, compositions, Geological occurrence, Zeolite synthesis, Aluminomsilicate gel, Crystalline mechanisms, Zeolites as ion exchangers, Zeolite catalysts, Interconversion of aromatics by Zeolites, Towards the future, Clays, pillared clays, and layered doublehydroxides.

6. **Ferroics :**Introduction, Proper and Improper ferroics, Primary and secondary Ferroics, Ferroelectrics, Relaxorferroics.

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 &ItsApplications*, 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-529 Nanochemistry

Course Objectives:

- To introduce and provide a broad view of the nascent field of nanoscience and nanotechnology to postgraduates
- To introduce students about the various techniques used to fabricate nanomaterial's from bulk materials
- To introduce students about techniques used to characterize nanpmaterials
- To provide the details of self-assembly and various advanced materials like nanocomposites
- To introduce students about organic nanomaterials (traditional and advanced) their properties
- To provide exposure of nanoelectronics and recent topics like molecular and DAN computing.

Course Content:

1. Introduction to Nanotechnology

Historical perspectives (History & Scope) of nanomaterials, Potentials of Nanotechnology in various sectors, classification of nanomaterialsetc. (**2 lectures)**

2. Methods of Generation of Nanomaterials

Introduction to Nanomaterials synthesis, Concepts of top-down and bottom-up approaches; physical (Arc discharge, laser ablation, aerosol, Inert gas condensation, High energy ball-milling, Chemical vapor deposition, plasma synthesis and Electro-deposition); Chemicals(Solvothermal,hydrothermal, Micro-emulsion, Sol-gel, Microwave, Sonochemical and co-precipitation method), Introduction and details of various types of Lithography, sputtering,

(10 Lectures)

3. Nanomaterials Characterization Techniques

Power X-ray diffraction (Scherrer equation),Electron microscopy (Introduction & Principal) including FE-SEM, TEM, and STM; AFM, XPS method of sample preparation of above mentioned techniques.

(10 Lectures)

4. **Self-Assembly**

Supramolecular&Dimension Control in Nanostructure, coded self-assembly, Superlattice.Nanocomposites& their applications (0**4 Lectures)**

5. Organic nanomaterials

DNA &Nanomaterials, Bionanocomposites, Biometrics, Molecular Motors, Molecular Machical Materials, used in diagnostic &therapetutic application (Gold nanoparticles, quantam dots) Fluorescent Biomarkers.CNT, Fullerenes their properties and applications.

(10 Lectures)

6. Nanoelectronics& Molecular computing

Molecular wires, Nanowires, Nanotubes,Molecular switches, Molecular logic gates, Molecular storage devices DNA & Quantum computing, dendrimers. (**04 Lectures)**

Course Outcomes:

1. The student will get exposure about the nanomaterials in present era
2. The student will get exposure about the various techniques used for fabrication of nanomaterials like physical and chemical methods
3. The students will get exposure about the various processes like self-assembly, superlattice etc.
4. The students will get exposure about various techniques used for the characterization of nanomaterials
5. The student will be able to understand about the organic nanomaterials like CNTs etc
6. The student will learn about recent topics like nanoelctronics, and DNA and molecular computing.

References:

1. The Chemistry of Nanomaterials: Synthesis, Properties and Applications, Rao, C.N.R., Müller, A. and Cheetham, A.K., , Vol. 1 and 2,Wiley-VCH Verlag, Weinheim.
2. Principals of Nanoscience& Technology,M A Shah &Tokeer Ahmad, by Narosa publication house New Delhi 2010
3. Introduction to Nanotechnology,C. P. Poole & F. J. Owens, Wiley,**2003.**
4. "Nanostructures and Nanomaterials: Synthesis, Properties and Applications",Cao, G. and Wang, Y., , 2nd Revised Ed., World
5. Nanotechnology, M. Wilson, K. Kannagara, G. Smith, M. Simmons &B. Raguse,CRC Press Boca Raton, 2002.

Prepared by Dr Uma Shanker **Rectified by: Dr N C Kothiyal**

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CY-530 Photochemistry

Course Objectives:

The aim of this course is to understand the basic principles and types of photochemical reactions. To ensure that students have a good knowledge about photo energy and solar energy conversion. To be aware with the significant applications of photochemistry in many life areas. Study the pericyclic reactions as the concerted reactions, which studies the mechanical reactions by thermal and photochemistry tools.

Course Content:

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 secondaryprocess.
2. **Determination of ReactionMechanism:**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 ofAlkenes:**Intramolecular reactions of the olefinicbond – 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 oxetaneformation.
5. **Photochemistry ofAromaticCompounds:** Isomerisation, additionsandsubstitutions.
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 ofvision.
7. **Inorganic Photochemical Processes:** Photosubstitution, rearrangement and redoxreacations.

Course Outcomes:

After completing the course the student should be able to

1. describe and explain common photochemical and photophysical processes and mechanisms with suitable theoretical models, and apply established experimental methods for the investigation of these processes
2. describe the interaction of excited states with their surroundings and analyse photoinduced electron transfer and excitation energy transfer with quantitative models

3. describe the structure and function of photosynthetic reaction centres, and explain the function of photosynthetic antenna systems
4. describe photo induced processes in semiconductors and at molecule-semiconductor interfaces, and explain how these can be used for photo physical energy conversion and in photo catalysis
5. describe and explain the environmental impact of atmospheric photochemistry, photoimage in biological systems, and therapeutic applications of photochemistry

References:

1. *Fundamentals of Photochemistry,* K. K. Rohtagi-Mukherjee, Wiley EasternLtd., **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**

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CY-531 Environmental Chemistry

1. **Chemistry of Atmosphere:** Composition, Chemical and photochemical reactions in the atmosphere, Ozone chemistry, Greenhouse effect, Global Warming.

2. **Air Pollution Monitoring:** Causes and Effects of air pollution, Sampling of gaseous pollutants and their Analysis, Monitoring of different air pollutants by U V Visible, IR, AAS and gas chromatographic methods, Monitoring of hydrocarbons by Gas Chromatography and GC-MS, Monitoring of fluorochloro carbons by gas chromatography and trace metal pollutants byAAS.

3. **Prevention and control of air pollution:** Source correction methods, Gaseous emissions, Adsorption by liquids, Adsorption by solids and combustion methods. Monitoring and control of automobileexhaust.

4. **Instrumental Method of water pollutants Monitoring and analysis:** Introduction to water pollution, cause, sources, Sampling techniques, Monitoring of different water pollutants, BOD, COD, DO analysis, Determination of TOS, Aromatic compounds by HPLC and GC methods., Methods of determination of TDS, SS, Alkalinity, Hardness, Monitoring of Anions by ion Selective electrodes method, Metal ions by AAS method, Monitoring of metalloids by spectrophotometermethods.

5. **Soil Pollution:** Source and causes of soil pollution, radio active pollutants, pesticides on soil, Role of micronutrients in soil-diseases caused by soil pollution, Control of soilpollution.

References:

1. *Waste water treatment disposal and release*-Metcalf and eddy, INC second Edn. Tata Mc Graw Hill,**1990.**
2. *Standard methods for the examination of water and waste water*-Andrew D. Eaton, Lenore, S. Clesceri and A. E. Greenberg, 19th Edn. EPS group, INC Roman,**1995.**
3. *Environmental pollution control and engineering* C. S. Rao, Wiley Eastern Ltd.,**1995.**
4. *Chemical and Biological methods for water pollution studeis*, R. K. Trivedy, and P. K. Goel, Environmental publications,**1986.**
5. *EnvironmentalChemistry*,B.K.Sharma&H.Kaur,GoelpublishingHouse, **1994.**
6. *Environmental Chemistry*, A. K. DE, 2nd edition, Wiley Eastern Ltd.,**1990.**
7. *Environmental Pollution Analysis*, S. M. Khopkar, Wiley Eastern Ltd.,**1995.**

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

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CY- 532 Statistical Thermodynamics

Course Objectives:

- To do direct theoretical calculation of physical (bulk, macroscopic) properties based on first-principles, statistical mechanics considerations
- To learns relevant macroscopic thermodynamic properties and relations
- Apply thermodynamic principles and the standard formulae to analyze thermal behavior of simple physical systems
- To derive partition functions for the various ensembles
- To obtain ideal gas and chemical equilibrium properties from partition functions

Course Content:

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

Course Outcomes:

Students will be able to

- compute various thermodynamic properties of idealized simple classical and quantum mechanical systems using standard techniques, such as the partition function and the grand partition function
- explain statistical physics and thermodynamics as logical consequences of the postulates of statistical mechanics;
- apply the principles of statistical mechanics to selected problems;

- apply techniques from statistical mechanics to a range of situations;

REFERENCES:

1. *Physical Chemistry*, P. Atkins, J. D. Paula, Indian Edition, Oxford,**2007.**
2. *Thermodynamics, Statistical Thermodynamics, and Kinetics*, T. Engeland 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
3 0 0 3

CY-533 Industrial Organic Chemistry

1. **Synthetic Dyes:** Introduction, Structural Features, Uses, Classification as per chemical constitution, Colour and constitution, classification based on application, Nito, Nitroso, Azo, Acid, Basic, Direct, Mordant, xanthenes, Heterocyclic and Sulphurdyes.

2. **Insecticides:** Brief Introduction and classification of insecticides and pesticides, chemical control of insects, Environmental friendly insecticides, uses andlimitations.

3. **Synthetic Polymers:** Introduction and uses of synthetic rubbers, plastics and fibers, conducting polymers, polymers in electronicindustries.

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 EmulsionExplosives.

6. **Synthetic Perfumes**: Introduction, chemistry anduses.

7. **Synthetic Drugs:** Introduction, Mechanism and drug action, Physiological activity and structures, Antimalarials, Sulpha Drugs, Metallic Therapeutics**,** SweeteningAgents.

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. RajeevJindal
3. Dr. JaspreetRajput

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CY-534 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 emulsionpolymerization.

3. **Types of Polymers:** Polymers with linear, branched and cross-linked structures, thermoplastic and thermosetpolymers.

4. **Molecular weight and distribution of polymers:** different methods of molecular weight determinations, colligative properties, viscometry, light scatteringtechniques

5. **Characterization of leather polymers:** TGA, DTA, DTG, XRD, FT-IR, SEM, TEM andDSC

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, cellulosics, Natural rubber processing andvulcanizing

7. **Fabrication of polymeric material:** compounding and mixing, casting , extrusion, fibre spinning, molding, coating and foamfabrication.

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 inpreservation.

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

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CY-535 Drug Design and Development

Course Objectives:

To prepare students for career as Quality professionals, providing the knowledge and skills required to ensure the safety of medicinal products worldwide.

Course Content:

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 ofdrugs.

2. **Drug Design and Development:** Screening of natural products-Isolation and purification-structure determination, structure activityrelationships

3. **Cimetidine: A Rational Approach to Drug Design:** Introduction, biological activity, metabolism, conformationalisomers

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 pharmacologicalactivity.

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 structuralinformation.

7. **Computer Assisted Molecular Modeling in Rational Drug Design.**

Course Outcomes:

At the end of this course, the students bring skills and knowledge related to formulation, quality management and testing of drugs in animals and peoples.

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.**

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CY-536 Mechanistic Inorganic Chemistry

Course Objective:

1. To understand ligand substitution reaction considering thermodynamic and kinetic aspects and their classification.
2. To study the mechanism of ligand substitution in square planar environment and application
3. To study the ligand substitution reactions in octahedral environment and their applications
4. To understand the mechanism of redox/electron transfer reactions: inner sphere and outer sphere mechanisms
5. To understand the mechanism of photochemical reaction and to study their application
6. To put light on heterogeneous, homogeneous catalysis and their important consequences.

Course Content:

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 andIsomerisation.

4. **Redox Reactions :** Classification, Inner sphere & Outer sphere mechanisms.

5. **Photochemical Reactions :**Prompt & delayed reactions metal-metal bond systems, d-d & charge transferreactions.

6. **Catalysis :**Heterogeneous**,** Homogeneous catalysis and their important consequences.

Course Outcomes:

Students will be able to establish a solid understanding on the mechanism involved for various inorganic reactions and they will be able to apply their concepts developed during the course to solve mechanistic problems of inorganic ligand substitution reaction, electron transfer reactions, photochemical reactions. They will also be able to understand and solve problems regarding heterogeneous and homogeneous catalysis.

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. *MechanismsofInorganicChemistry*,F.BasoloandR.G.PearsonWiley, **1967.**

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

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CY-537 Advanced Organic Chemistry

Course Objectives:

1. To predict the relationships between organic chemical structures, their reactivity and use of reagents in regioselective, chemoselective and enantioselective synthesis.
2. To learn the advanced concepts in organic synthesis along with newly established organic name reactions.
3. To predict and account for the most commonly encountered reaction mechanisms in organic chemistry.
4. To study the various rearrangement in organic chemistry.

Course Content:

1. **Metal and Non-metal mediated oxidation and reductions:** Mechanism, selectivity, stereochemistry and applications of Chromium, Manganese, Silver, Ruthenium, DMSO, TEMPO, and iodine based reagents (IBX, Dess-Martion Periodinate); DDQ, Swern oxidation, Pd, S and Se catalysed dehydrogenation. Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Clemmensen reduction, Wolff-Kishner reduction, Dissolving metal reductions, metal hydride reductions using DIBAL. Boron in reduction. (10 Lectures)

2. **Rearrangements:** A detailed study of the following rearrangements: Benzil-Benzillic acid, Arndt-Eister syntheses, Neber rearrangement, Shapiro reaction, Carroll, Gabriel–Colman, Smiles rearrangement, Stevens and Sommelet–Hauser rearrangements. **(10 Lectures)**

3. **Reagents in organic synthesis:** Gilman's reagent, Lithium diisopropylamide (LDA), Dicyclohexyl Carbodiimide (DDC), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Bakers yeast, Prevost Hydroxylation, Merifield resin, Ziegler-Natta catalyst, Lawson reagents, K-selecteride and L-selecteride, Sodium cyanoborohydride, 9-BBN, Manganese dioxide, Dioxiranes, Ceric ammonium nitrate, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent. Use of Cu, B, Mg, Li, Zn, Si, Os, Ru, and Tl reagents inorganic synthesis. **(10 Lectures)**
4. **New Synthetic Reactions:** Baylis-Hillman reaction, Biginelli reaction, Mukaiyama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's olefination, Buchwald-Hartwig coupling, Shapiro reaction, Stork-enamine reaction Aza-Cope, Aza-Wittig reaction, BINAL and BINAP assisted reactions. Ugi reaction, Robinson–Gabriel synthesis, Strecker amino acid synthesis, Vilsmeier–Haack reaction, Wohl–Ziegler reaction. **(10 lectures)**

Course Outcomes:

At the end of the course, the student will be able

1. To study the various reagents used in organic chemistry for regioselective, chemoselective and enantioselective multi-step synthesis

2. To predict the relationships between organic chemical structures and their reactivity and further transformations.

3. To learn the fundamental and advanced concepts in reaction mechanisms in organic chemistry along with the study of reaction mechanisms in various types of newly discovered reactions.
4. To study the new methodologies for altering the reactivity patterns of organic molecules and synthesize molecules using combinations of different reagents

References:

1.Organic chemistry, Claydon, J., Gleeves, N., Warren, S., Wother, P.; (2001), Oxford University Press, UK.

2.Name Reactions: A Collection of Detailed Reaction Mechanism, Li, J.J., (2009). Springer, 4th edition.

3.Advanced organic chemistry: Reaction Mechanism, Bruckner, R., (2001). Elsevier, 1st edition.

4.Advanced Organic Chemistry Part A and Part B Carey, B. F. A., Sundberg R. J., (2007). Springer, 5th edition.

5.Some Modern Methods of Organic Synthesis, Carruthers, W., (2004). Cambridge Uni.Press, 4th edition.

6.Organic Synthesis: Special Techniques, Ahluwalia, V. K., Aggarwal R., (2001). Alpha Science, New Delhi.

7.Reagents for organic synthesis, Fieser and Fieser, (2011). Vol 1-26.Wiley Interscience,3rd edition.

8.Organic Chemistry,Finar, I. L., (2012). Pearson Education, 6th edition, UK.

9.A text book of Organic Chemistry, Bansal, R.K., (2012). New Age Inrternational (P) Ltd., 4th edition New Delhi.

10. Advanced Organic Chemistry, Reactions Mechanisms and Structure, March, J., (2007) John Wiley, 6th edition.

11. Handbook of Reagents for Organic Synthesis Acidic andBasic Reagents VoI.Reich, H. J., Rigby, M., (1999). IV Wiely-Interscience

12. Organic synthesis: The Synthon Approach.Warren, S., (2010). John wiley & Sons, NewYork.

13. Designing organic synthesis: A Disconnection Approach Warren, S., (2010).. John Wiley and Sons, New York.

Prepared by Dr Virender Singh and Dr Uma Shanker Rectified by Dr Jaspreet Kaur and Dr Rajeev Jindal

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List of Open Elective Courses for B. Tech/ M.Tech/Ph D Students

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CYOE-401 Molecular Electronic Devices

1. **Introduction:**Background, Justification andprospects.

2. **MolecularelectronicDevices:**Advantageofmoleculesas electronic devices molecular design and constrains of moleculardevices.

3. **MolecularWires:**Synthetic routes to design of molecular wireandtheirtesting.

4. **Molecularswitches:**Alternativeswitchingmethodologies,molecules as switches.

5. **MolecularLogicGates:**Strengths of molecules as logic gates,examplesof molecular logic gates and theirapplications.

6. **Molecular StorageandTransport:**Design of molecules for storageandtransport, methodologies andlimitations.

7. **MolecularSuperconductors:**Molecular approachtowards superconductivity, molecular magnetism and theircorrelation.

8. **QuantumComputers:**Molecular approach towardscomputing,quantumcomputing, DNA computing and theirlimitations.

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

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CYOE-402 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 theirapplications in differentfields.

3. **Molding Techniques:** Introduction, different molding techniques (both for Thermosetting and thermoplastic resins), additives and their functions, applications of different moldingtechniques.

4. **Conducting Polymers:** Introduction, classification, different types of dopings, synthesis, applications in differentfields.

5. **Composites:** Introduction, classification, different types of reinforcing materials and their applications, failure modes, advantages andapplications.

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

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CYOE-403 Nanoscience and Nanotechnology

1. **Introduction** : Nano science, Nano technology, history and scope.

2. **Characterization & Fabrication:** Contemporary Characterization Methods, Top down & Bottom up Fabrication, Solution based Synthesis of Nanoparticles, Vapour Phase Synthesis & Synthesis with framework.

3. **Lithographyand Chemical Patterning:** Nanolithography, Dip Pen Lithography, e-beam lithography, Nanospherelift off lithography.

4. **Quantum Structures:** Quantum Well, Quantum wires, Quantum Dots, Super lattices & Layered Structures, Quantum Computing.

5. **Self Assembly:** Supramolecular& Dimension Control in Nanostructure, thermodynamic and coded self assembly.

6. **Carbon Nanostructures and Biomaterials:** Carbon molecules, clusters, carbon nanotubes and their applications DNA &Nanomaterials,Bionanocomposites, Biometrics, molecular motors.DNA Computing.

7. **Nanoelectronics:** Molecular wires, Molecular switch, Molecular logic gates and molecular storage devices, Nanowires, Nanotubes.

Recommended Books:

1. C P Poole & F J Owens *Introduction to Nanotechnology*, **2003**, Wiley.
2. M Ratner & D Ratner *Nanotechnology*, **2003**, Prentice Hall.
3. M Wilson, K Kannagara, G Smith, M Simmons & B Raguse *Nanotechnology*, **2002**, CRC Press..
4. Geoffery A Ozin& Andre, C. Arsenault *Nanochemistry, A Chemical approach to Nanomaterials*, **2005,** Royal society of Chemists.
5. Lynn E. Foster *Nanotechnology, Science Innovation & Opportunity*, **2007**, Pearson Education.

List of Courses Exclusively for Ph D Students

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3 1 0 4

CY-538 Green Chemistry

Unit-I

Introduction to green chemistry: Basic principles of green chemistry: Atom economy and scope, Prevention/Minimization of hazardous/toxic products, Designing safer chemicals, Selection of appropriate auxiliary substances (solvents, separation agents etc), use of renewable starting materials, Avoidance of unnecessary derivatization-careful use of blocking/protection groups. Use of catalytic reagents in preference to stoichiometric reagents, Designing biodegradable products, Prevention of chemical accidents, Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

Unit-I

Approaches to green synthesis: Use of green reagents in green synthesis: polymer supported reagents, polymer supported peptide coupling reagents. Green catalysts, Phase-transfer catalysts in green synthesis. Advantages of PTC, Reactions to greensynthesis, Application of PTCs in C-alkylation, N-alkylalion, S-alkylation.Darzensreaction, Williamsons synthesis, Wittig reaction. Use of Crown ethers in esterification,saponification, anhydride formation, aromatic substitution and elimination reactions.
Ionic liquids as green solvents.

Unit III

Microwave induced and ultrasound assisted green synthesis: Introduction to syntheticorganic transformation under microwave (i) Microwave assisted reactions in water and organic solvents. (ii) Microwave assisted solvent free reactions. Ultrasound assisted reactions: Introduction, substitution reactions, addition, oxidation,reduction reactions. Biocatalysts in organic synthesis: Introduction, Biochemicaloxidation and reductions.

Unit IV

Organic synthesis in aqueous phase and in solid state: Solid statereactions (i) Solid phase synthesis without using any solvent (ii) Solid supportedsynthesis.

Suggested readings:

1. Ahulwalia, V.K.; Kidwai M. (2004). *New Trends in Green Chemistry*, Springer
2. Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical*. OxfordUniversity Press.
3. Grieco, P.A. (1997). *Organic Synthesis in Water*. Publisher: Kluwer Academic.

Prepared by Dr Virender Singh
Rectified by Dr Uma Shanker and Dr JaspreetKaur Rajput

L T P C
3 1 0 4

CY-539 Principles of Instrumental Methods of Analysis

Course Objectives:

To develop skills of students in instrumentation and biological techniques

Course Content:

1. **Data Handling :** Introduction ,Sensitivity and Detection limit, Noise and sources, Uncertainties, Errors, calibrations, Mean, Standard Deviation , Least square fit, computer aidedanalysis
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 ,Thermometrictitrations
3. **Gas Chromatography :** Classification of chromatographic methods, Principles of Gas Chromatography, plate theory, Instrumentation, Working, Applications, Gas SolidChromatography
4. **High Performance LiquidChromatography:**Principle,Instrumentation, Supports in HPLC, Applications of HPLC systems, Supercritical fluid Chromatography (SFC), Recent developmentsinSFCandApplications
5. **Exclusion Chromatography :**Gel permeation Chromatography, Applications of GPC, Ion Exclusion, Mechanism of ion exclusiontechnique.
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 andPolarography
8. **Modern Methods of Surfaces Analysis :**Basic principle ,Instrumentation and applications of SEM, TEM andAFM.

Course Outcomes:

At the end of this course, the students would have learnt about principles of spectroscopy, & chromatography and all biotechniques.

References:

1. *Instrumental Methods of Analysis*, Willard, Merritt, Dean and Settle, CBS Publisher andDistributors.,**1986.**
2. *Thermal Analysis,* W. W. Wendlandt and L. W. Collins, Dowden Hutechin and Ross.
3. *Basic Concepts of Analytical Chemistry*, S. M. Khopkar , WileyEastern
4. *Thermal Methods of Analysis,* Principles, Application and Problems, J. Haines,

Blackie Academic and Professional,**1994.**

5. *Chromatographic Methods*, A. Braithwaite and F. J. Smith, 5th edn. Blackie Academic and Professional, London,**1996.**
6. *Principles of Instrumental Analysis*, Skoog, Holder, Nieman, Fifth edition Thomson Books,**1998.**

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

L T P C
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CY- 540 Advanced Spectroscopy

Course Objective:
The objectives of this subject are to provide students with an increased knowledge and understanding of advanced chemical principles, with emphasis on:

1. background spectroscopic theory
2. The use of instrumentation
3. analysis of experimental spectroscopic data

Course Content:

1. **Ultraviolet and VisibleSpectroscopy:**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 inbiphenyls.

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 forketones.

4. **Nuclear Magnetic ResonanceSpectroscopy:**General introductionand 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 othernuclei-F,P.

5. **Carbon-13 NMRSpectroscopy:**Generalconsiderations, chemicalshift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INADEQUATEtechniques.

6. **Mass Spectroscopy :**Introduction, Ion production & detection – El, Cl, 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.

Course Outcomes:

After completion of this course students will be able to interprete spectra which will help them to analyze inorganic and organic compounds. The combination of background theory and range of examples will enhance students' ability to acquire and analyze experimental data.

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.

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CY-541 Chemistry of Materials

Course Objectives:

1. To impart knowledge of synthesis and formation of various materials.
2. To provide knowledge to acquire the interrelationships between structure, processing and properties of materials.
3. To introduce the fundamental concepts and core techniques of design and testing of materials for taking different challenges in R & D.

Course Content:

1. Multiphase Materials:

Ferrous alloys , Fe-C phase transformations in ferrous alloys , stainless steels, non-ferrous alloys , properties of ferrousand non-ferrousalloysandtheirapplications.

2. Glasses, Ceramics and Composites:

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

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, molecularorderingin different mesophases ,identificationof liquidcrystals , polymeric liquid crystals , applications of liquid crystals indisplays and inthermography.

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– opticalproperties, ferromagnetism and some unusual properties offullerenes.

Course Outcomes:

Students should be able to reach the following goals upon the completion of the course:

1. To generate a solid understanding of the fundamental knowledge of materials science in particular the fundamental theories of methods and tools on the synthesis and characterization of Material Chemistry,
2. To get a preparation for the ability on materials design and R&D.
3. To develop and improve problem solving skills in scientific research using gain knowledge and methodology of materials chemistry.

References:

1. *SolidStatePhysics*,N.W.AshcroftandN.D.Mermin,SaundersCollegeEd. **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, CRCPress, Ed.**2007.**

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CY-542 Macromolecular Chemistry

Course Objectives:
To introduce the student to

1. General Introduction

(i) Historical, scope & emphasis.

(ii) Nomenclature, terms and definitions.

(iii) Overview of polymer types, structures, properties and methods of formation.

2. Polymer Molecular Weights

(i)Definitions and terms.

(ii)Measurement of polymer molecular weights.

3. Step-growth Polymerization

(i)Introduction.

(ii)Mechanism and kinetic analysis.

4. Free Radical Polymerization

(i)Introduction.

(ii)Mechanism and kinetic analysis.(iii)Co-polymerization - mechanism and kinetic analysis.

5. Other Polymerization Mechanisms

(i)Introduction.

(ii)Cationic, Anionic, Ziegler-type.

(iii)Polymerization methods. — practical aspects.

6. Polymer Structures and Stereochemistry

(i)Introduction - terms

(ii)Characterization of polymer structure and stereochemistry by physical methods, most importantly NMR spectroscopy.

Course Content:

1. **Basics:** Basic concepts: Monomers, repeat units, functionality,degreeof polymerization, classification, types of polymerizations, different types of initiators, polymerization in homogeneous and heterogeneous systems and importance ofpolymers.
2. **Polymer Characterization:**Polydispersion: Averagemolecularweight 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 abrassionresistance.

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 polymerdegradation.
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 transfermoulding.
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 bloodcells.

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, PrenticeHall. 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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