MOTHER TERESA WOMEN'S UNIVERSITY

Department of Chemistry

(Under Choice Based Credit System - CBCS)

(FOR THE CANDIDATE TO BE ADMITTED FROM THE ACADEMIC YEAR 2018-19)

Mother Teresa Women's University

Kodaikanal

PROGRAMME EDUCATIONAL OBJECTIVES (PEO)

The Post Graduates of M.Sc. Chemistry Programme will be able to

PEO1: Apply chemical principles and theories and acquire skills in synthesis, instrumentation and characterization.

PEO2: Apply laboratory skills and critical thinking to develop applications for solving Industry oriented problems.

PEO3: Function as a team member and develop projects in a multi-disciplinary environment by emulating leadership skills.

PEO4: Work productively as chemistry professional by adopting to environment with lifelong learning and adhering to ethical standards and apply the knowledge acquired for the improvement of the society.

PROGRAMME OUTCOMES (PO)

The M. Sc Chemistry programme is designed in such way to make the learners

1. Understand and appreciate the importance of Chemistry as a central science by the knowledge of its diverse applications.
2. Have sound knowledge of the fundamental and advanced concepts of applications of chemical and scientific theories.
3. Acquire experimental skills required for employment in chemical and pharmaceutical industry.
4. Develop analytical and problem-solving skills
5. Acquire the ability to synthesize, separate and characterize compounds using laboratory and instrumentation techniques.
6. Identify the major problems of the society and environment for which Chemistry has offered and can provide solutions and get motivated to further work on it by pursuing research with social responsibility.

PROGRAMME SPECIFIC OUTCOMES (PSO)

At the completion of the M.Sc. Chemistry program, the students will be able to:

PSO-1 Apply the knowledgeacquired about chemical reactions and their mechanisms to design new synthetic pathways

PSO-2 Design and synthesize new compounds which have potential applications in Industry and Medicine.

PSO-3 Carry out experiments and analysis in the area of organic analysis, estimation, separation, inorganic semi micro analysis, preparation

PSO-4 Apply the concepts and applications of kinetics thermodynamics
,
PSO-5 Open up new methods for environmental pollution&apply green/sustainable chemistry approach towards planning and execution of research in frontier areas of chemical sciences

PSO-6 Deduce the structure of compounds using various characterization techniques

PSO 7 Analyze& appreciatethe different types polymers, supramolecular materials, naturally available chemicals and their synthetic congeners

PSO-8 Apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories

PSO-9 Perform estimation experiments relating to electrochemistry, thermodynamics and Kinetics

PSO-10 Apply the concepts of quantum mechanics and group theory

MOTHER TERESA WOMEN'S UNIVERSITY
KODAIKANAL – 624 101
M.Sc. Chemistry Syllabus
Papers offered in each semester – Scheme of Examination

Paper No.	Paper Code	Course Title	Hours/ Credits	Continuous internal Assessment (CIS)	End Semester Exam (ESE)	Total
SEMESTER – I						
1	PCHT11	Organic Chemistry I	5/5	25	75	100
2	PCHT12	Inorganic Chemistry I	5/5	25	75	100
3	PCHT13	Physical Chemistry I	5/5	25	75	100
4	PCHP11	Organic Chemistry Practical	5/5	25	75	100
5	PCHE11	Medicinal Chemistry and Drug Design	5/5	25	70	100
		Total	25			500
SEMESTER –II						
6	PCHT21	Organic Chemistry II	5/5	25	75	100
7	PCHT22	Inorganic Chemistry II	5/5	25	75	100
	PCHT23	Physical Chemistry II	5/5	25	75	100
8	PCHP22	Inorganic Chemistry Practical	5/5	25	75	100
9	PCHE22	Analytical Techniques	5/5	25	75	100
	Total		25			500
SEMESTER – III						
11	PCHT31	Organic Chemistry III	5/5	25	75	100
12	PCHT32	Inorganic Chemistry III	5/5	25	75	100
13	PCHT33	Physical Chemistry III	5/5	25	75	100
14	PCHP33	Physical Chemistry Practical	5/5	25	75	100
15	PCHE33	Environmental Chemistry and Green Chemistry	5/5	25	75	100
	Total		25			500
SEMESTER – IV						
16	PCHT41	Chemistry of Natural Productsand Bioinorgnaicchemistry	5/5	25	75	100
17	PCHT42	Nanochemistry &Supramolecular Chemistry	5/5	25	75	100
19	PCHP43	Project Work	5/5	40	60	100
		Total	15			300
	Total		90			1800
90						

AVERAGE PERCENTAGE OF THE COURSES HAVING FOCUS ON SKILLS

Courses	Employability	Skill	Ent*	Knowledge
PCHT11 -ORGANIC CHEMISTRY-I	Y	Y		Y
PCHT21 - ORGANIC CHEMISTRY-II	Y	Y		Y
PCHT31 -ORGANIC CHEMISTRY-III	Y	Y		Y
PCHT12- INORGANIC CHEMISTRY I	Y	Y		Y
PCHT22- INORGANIC CHEMISTRY II	Y	Y		Y
PCHT32 – INORGANIC CHEMISTRY III	Y	Y		Y
PCHT13- PHYSICAL CHEMISTR I	Y	Y	Y	Y
PCHT23- PHYSICAL CHEMISTR II	Y	Y	Y	Y
PCHT33- PHYSICAL CHEMISTR III	Y	Y	Y	Y
PCHE11- MEDICINAL CHEMISTRY AND DRUG DESIGN	Y	Y	Y	Y
PCHE22- ANALYTICAL TECHNIQUES	Y	Y	Y	Y
PCHE33- ENVIRONMENTAL CHEMISTRY AND GREEN CHEMISTRY	Y	Y		Y
PCHT41- CHEMISTRY OF NATURAL PRODUCTS AND BIOINORGANIC CHEMISTRY	Y	Y		Y

SEMESTER – I

PCHT11 ORGANIC CHEMISTRY – I 5/5

Objectives

1. To make the students appreciate the importance of different types of reactive intermediates in organic reactions.
2. To provide understanding of the different types and mechanism of organic reactions
3. To make the students understand and appreciate the basic concepts of stereochemistry
4. To provide understanding of the concept of aromaticity and enable the students to identify aromatic, non-aromatic and anti-aromatic compounds.

Course Outcomes
Upon completing the course, the students will be able

1. Identify the different types of reactive intermediates and appreciate their importance in organic reactions
2. Understanding the various mechanisms of organic reactions
3. Understand and apply the concepts of stereochemistry
4. Identify aromatic, non-aromatic and anti-aromatic compounds

Unit I

Reactive intermediates and Aromaticity

Carbocations, carbanions, carbenes, benzynes and nitrenes-Generation, stability and reactivity.

Aromatic character: Six-, five-, seven-, and eight- membered rings - Other systems with aromatic sextets – Huckel's theory of aromaticity, concept of homoaromaticity and antiaromaticity, Electron occupancy in MO's and aromaticity - NMR concept of aromaticity and antiaromaticity, systems with 2,4,8 and 10 electrons, systems with more than 10 electrons, alternant and non-alternant hydrocarbons (azulene type). Bonding properties of systems with (4n+2)□□electrons and 4n□□electrons, Heteraromatic molecules. Annulenes, heteroannulenes, sydnones and fullerenes. Craig's rule, Hammond's postulate

Unit II

Substitution reactions

Nucleophilic Substitution

1. Aliphatic nucleophilic substitution: S_N1 and S_N2 mechanism – Kinetic and stereochemical characteristics – effects of substrate structure, nature of the nucleophile

and leaving group on the rate – solvent effects – examples of S_Ni substitution – Neighbouring group participation-Anchimeric assistance

2. Aromatic nucleophilic substitution: Benzyne and Meisenheimer intermediates

Electrophilic Substitution

1. Mechanism of aliphatic electrophilic substitution reaction – S_E1, S_E2, S_Ei reaction.

2. Mechanism of aromatic electrophilic substitution reactions – complexes – nitration, halogenation, sulphonation, Friedel Craft alkylation and acylation – Reimer Tiemann reaction. Linear free energy relationship – Hammett equation – Significance of the σ and ρ parameters; Taft equation.

Unit III

Addition and Elimination reactions

Addition reactions
Regio and stereochemistry of addition of halogens and halogens acids to carbon – carbon multiple bonds – hydroboration – addition to carbonyl bonds – mechanism of Aldol, Perkin, Stobbe, Dieckmann condensation, Reformatsky and Grignard reaction, Michael addition reaction and Mannich reaction – Formation and Synthetic application of enamines – Stork enamine reaction.

Elimination reactions
E1, E2, E1CB mechanism – structural and solvent effect on these mechanisms – orientation of double bonds (regio and stereoselectivities) – competition between substitution and elimination reaction – cis elimination, pyrolytic eliminations

Unit IV
Rearrangements

Definition – nucleophilic, electrophilic and free radical rearrangements – intramolecular and intermolecular rearrangements – migratory aptitude – Wagner – Meerwin, Benzil – Benzilic acid, Schmidt, Lossen, Curtius, Beckmann, Fries, Baeyer Villeger, Favorski, Stevens and Neber rearrangements.

Unit V

Introduction to stereochemistry

Concept of chirality: specification on configuration by Cahn, Ingold and Prelog system of notation, compounds with more than one chiral centre – calculation of number of stereisomers –

erythro and threo nomenclature; interconversions of Sawhorse, Fisher and Newman's Projections.

The concept of prochirality: Topicity and prostereoisomerism – equivalent, enantiotopic and diasteriotopic ligands and faces. Atropisomerism – concept of axial chirality 'R' and 'S' nomenclature of some axially chiral molecules.

Geometrical isomers – E & Z nomenclature determination of configuration of geometrical isomers by physical and chemical methods.

Text books

1. J.March, Advanced Organic Chemistry, 4thEdn. John Wiley, New York,1992.
2. P.Sykes, A Guide book to Mechanisms in Organic Chemistry, 6thEdn., Longmans Scientific and Technical, Essex, 1986.

Reference Books:

3. F.S.Gould, Mechanism and Structure in Organic Chemistry, Holt, New York,1959.
4. T.H.Lowry and K.S.Richardson, Mechanism and theory in Organic Chemistry, Harper and Row, New York, 1976.
5. T.W.G.Solomons, Organic Chemistry, 6thEdn., John Wiley, New York, 1996.
6. G.W.Loudon, "Organic Chemistry", 3rdedn. Benjamin-Cummings, 1995.
7. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part A and Part B, 3rd Edn., Plenum press, New York, 1990.

Mapping of Cos with POs &PSOs:

PO/PSO	PO 1	PO 2	PO 3	PO 4	PO 5	PO6	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO6	PSO 7	PSO 8	PSO 9	PSO10
CO1	S	S	M	S	M	M	S	S	M	M	M	M	M	M	M	M
CO2	S	S	M	S	M	M	S	S	M	M	M	M	M	M	M	M
CO3	S	S	M	S	M	M	S	M	M	M	M	M	M	M	M	M
CO4	S	S	M	S	M	M	S	S	M	M	M	M	M	M	M	M

Strongly Correlating(S) - 3 marks
Moderately Correlating (M) - 2 marks
Weakly Correlating (W) - 1 mark
No Correlation (N) - 0 mark

PCHT12 INORGANIC CHEMISTRY – I 5/5

Objectives:

1. To provide knowledge of basic and advanced concepts in bonding and enable the students to identify the structure and bonding of simple molecules.
2. To provide an understanding of the various types of solid state packing and the types of chemical forces
3. To provide knowledge of the structure and bonding of main group elements and their compounds
4. To provide a basic knowledge of the polymeric inorganic compounds.

Course Outcomes:

On learning the course, the students will be able to

1. Understand the principles of various bonding theories and identify the structure and bonding of simple molecules.
2. Recognize the various types of solid state packing and the types of chemical forces
3. the structure and bonding of main group elements and their compounds
4. to appreciate the existence and application of polymeric inorganic compounds

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Unit I

Covalent Bonding

V.B. approach to bonding-Hitler-London, Pauling and Slater refinements, Concept of hybridization and structure of molecules, VSEPR theory shapes of molecules. M.O. approach to covalent bonding – symmetry and overlap of atomic orbitals – symmetry of molecular orbitals – sigma, pi and delta bondings – energy levels in homo and hetero nuclear diatomic systems – bond length, bond order and bond energy, Application to small molecules such as $BeCl_2$, BCl_3 and CCl_4, SF_4, ionic character in a covalent bond. The concept of multicentre bonding.

Unit II

Metallic Bonding

Drude Lorentz theorem, merits and demerits – Sommerfieldtheroem – band theorem – formation of Brillion Zones – conductors and insulators and semiconductors, – Hall effect – super conductors, photoconductivity. Point-, line- and plane defects in solids – Stoichiometric and non-stoichiometic defects – Frenkel and Schottky defects.Effect of imperfections on physical properties like electrical conductivity, thermal, optical and magnetic phenomena.

Unit III

Solid State – Structure

Cohesive energy and Medelung constants, Van der Waals forces, Close packing of atoms and ions HCP and BCC types of packing voids, radius ratio – derivation – its influence on structures. Lattice energy – Born-Lande equation - Kapustinski equation.Representative structures of AB and AB_2 types of compounds - rock salt, cesium chloride, wurtzite, zinc blende, rutile, fluorite, antifluorite, cadmium iodide and nickel arsenide.Structure of graphite and diamond.Spinels -normal and inverse types and perovskite structures.

Unit IV

Main Group Chemistry

Chemistry of boron – borane, higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon – silanes, higher silanes, multiple bonded systems, silicon nitrides, siloxanes. P-N compounds, cyclophosphazenes and cyclophosphazanes. S-N compounds – S_4N_4, $(SN)_x$.

Unit V

Interhalogens and Polymeric Inorganic Compounds

Pseudo halogens; , Structure and bonding in ClF_3, BrF_3 , BrF_5 , IF_5, IF_7 etc . Oxides and oxoacids of halogens, Isopoly and heteropoly acids – Structure and bonding of 6- and 12 – isopoly andheteropoly anions. Structure of silicates - applications of Paulings rule of electrovalence - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three dimensional silicates – Bonding in Noble gas compounds – $XeCl_2$, XeF_4, $XeOF_4$, XeF_6.,

Text Books

1. J.E. Huheey, Inorganic Chemistry, 3rd. Ed., Harper & Row publisher, 1983.
2. J.D. Lee, Concise Inorganic Chemistry, 5th Ed, Wiley, 1999.
3. William Jolly, Advanced Inorganic Chemistry

Reference Books

1. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed. 1994.
2. M.C. Day, J. Selbin, Theoretical Inorganic Chemistry, 2nd Ed., East West Press, 1985.
3. F. Basolo, R.G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., John Wiley, 1967.
4. L. Pauling, The Nature of the Chemical Bond, 3rd Ed., Cornell University Press, 1960.
5. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4th Ed., John Wiley & Sons, 1986.
5. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, 3rd Ed, 1999.
6. A.G. Sharpe, Inorganic Chemistry, Pearson Education, 2008.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
CO1	S	S	M	S	M	M	M	S	M	M	M	M	M	M	M	M
CO2	S	S	M	S	M	M	M	S	M	M	M	M	M	M	M	M
CO3	S	S	M	S	M	M	M	S	M	M	M	M	M	M	M	M
CO4	S	S	M	S	M	M	M	S	M	M	M	M	M	M	M	M

PCHT13 PHYSICAL CHEMISTRY - I 5/5

Objectives:

1. To enable the students to understand concept and laws of thermodynamics
2. To understand and appreciate the advanced concepts and rate equations in chemical kinetics.
3. To provide knowledge on the concepts and laws of electrochemistry and photochemistry
4. To enable the students to apply the knowledge gained in the above concepts

Course Outcome

On learning the course, the students will be able to

1. Calculate change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential.
2. Identify factors affecting equilibrium constant.
3. Understand and appreciate the advanced concepts and rate equations in chemical kinetics.
4. Understand and apply the concepts and laws of electrochemistry and photochemistry

Unit I

Thermodynamics Chemical and Phase Equilibrium

The second law of thermodynamics – Entropy – thermodynamics of systems of variable compositions – partial molar quantities and their determination – chemical potential – Gibbs-Duhem equation – Activity and Fugacity- determination of fugacity, Nernst equation, Third law of thermodynamics, exceptions and applications. Chemical equilibrium - temperature dependence, Vant-Hoff equation, Non-equilibrium thermodynamics - postulates and methodology. Phase equilibrium-Application to three component system-CH_3COOH, H_2O and $CHCl_3$ system.

Unit II

Chemical Kinetics

Derivation of rate constant for opposing, consecutive and parallel reaction-steady state approximation. Chain reactions: kinetics of decomposition of N_2O_5 – Non stationary chain reaction: H_2O_2 reaction and explosion limits. Grunwald –Winstein equation on reaction rates.Concept of Linear Free Energy Relationships-derivation of Hammett equation-significance of substituent and reaction rate constants - Taft equation - thermodynamic implications of LFER.Experimental methods for the study of fast reaction-flow method-relaxation methods.

Unit III

Electrochemistry – I

Mean ion activity and activity coefficient of electrolytes in solution – Ion association - Ionic strength – Debye-Huckel theory – Debye-Huckel limiting law - its validity and limitations – Strong and weak electrolytes – Debye theory of electrolytic conductance – Debye – Huckel – Onsager equation - Verification and limitations - Electrochemical cells and applications of

standard potentials. Batteries-Primary and secondary fuel cells – Corrosion and corrosion inhibition

Unit IV

Electrochemistry – II

The electrical double layer – Polarizable and non-polarizable interfaces – Structure of electrical double layer – Electrocapillary and double layer capacity measurements – Double layer models – Helmholtz, Guoy–Chapman and Stern models.

Electrokinetic phenomena: Zeta potential – Electrophoresis Electroosmosis, sedimentation potential and streaming potential, Kinetics of electrode processes – Current–potential curve – Butler–Volmer relation and its approximations – Tafel equation – Charge transfer resistance – Nernst equation from Butler–Volmer equation –Multistep processes – Symmetry factor and transfer coefficient – Electrocatalysis–Hydrogen evolution reaction as a case study.

Unit V

Photochemistry

Absorption of light by molecules, reaction paths of electronically excited molecules – de-excitation pathways, Fluorescence and Phosphoresence – Jablanski diagram – Physical properties of the electronic excited molecules – excited state dipole moments, excited state pKa and redox potentials – Stern – Volmer equation and its application – photosensitization – Chemi Luminescence – Quantum Yield and actinometry.

Text Books

1. P.W. Atkins,Physical Chemistry, 7th Ed., Oxford University press, 2002.
2. J. Rajaram and J.C. Kuriacose, 2nd Ed., Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, ShobhanLalNagin, New Delhi, 1996.
3. G.W.Castellan, Physical Chemistry, Narosa, 1996.
4. K.J. Laidler, Chemical Kinetics, 3rd Ed., Pearson Education, 2004.
5. S. Glasstone, Text book of Physical Chemistry, McMillan, 1974.
6. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, New Age International, 2000.

Reference Books

1. J. Moore, Physical Chemistry, 5th Edn., Orient Longman.1972
2. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, 1969.
3. I.M. Klotz, P.M. Rosenberg, Chemical Thermodynamics: Basic Concepts and Methods, 7th Ed., John Wiles & Sons, 2008.
4. A.A. Frost, R.G.Pearson, Kinetics and Mechanism, John Wiley & Sons, 1953.
5. J.I. Steinfeld, J.S.Francisco, W.L. Hase, Chemical Kinetics and Dynamics, 2nd Ed, Prentice Hall, 1999.
6. K.S. Gupta, Chemical Kinetics and Reaction Mechanism , RBSA Publishers, 1992.
7. A.J. Bard, L.F. Pahlkner, Electrochemical methods – Fundamentals and applications, 2nd Ed., Wiley-VCH, 1998.
8. J. Albery, Electrode kinetics, Clarendon Press, Oxford Chemical Series, 1979.
9. D.R.Crow, Principles and applications of Electro Chemistry, Chapman & Hall.
10. D.A. McQuarrie, D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt. Ltd, 2003.
11. J.O. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Ed., Springer, 2006.
12. L.I. Anthrapov, Theoretical Electrochemistry, Mir Publishers, Moscow, 1972.
13. P.H. Rieger, Electrochemistry, Prentice-Hall, Inc, 1987.
14. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry,New Age International, 2000.
15. N.J. Turro, Molecular Photochemistry, W. A. Benjamin, 1966.
16. J.R. Lakowicz, Principles of fluorescence spectroscopy, Springer, 2006. C.H. Hamann, A. Hammett, W. Vielstich, Electrochemistry, Wiley-VCH, 1998.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
CO1	S	S	M	S	M	M	S	M	M	S	M	M	M	M	S	S
CO2	S	S	M	S	M	M	S	M	M	S	M	M	M	M	S	S
CO3	S	S	M	S	M	M	S	M	M	S	M	M	M	M	S	S
CO4	S	S	M	S	M	M	S	M	M	S	M	M	M	M	S	S

PCHP11 ORGANIC CHEMISTRY PRACTICALS 5/5

Objectives:

1. To develop understanding in basic chromatographic methods.
2. To learn simple extraction techniques
3. To develop skill in simple organic synthesis
4. To understand and develop the principles of quantitative and qualitative analysis of organic compounds.

Course Outcomes

On learning the course, the students will be able to

1. Understand in basic chromatographic methods.
2. Learn simple extraction techniques
3. Develop skill in simple organic synthesis
4. Understand and develop the principles of quantitative and qualitative analysis of organic compounds.

1. Purification techniques of organic compounds and their spectroscopic identifications.
   a) Purification of binary mixtures by Thin Layer Chromatography (TLC) and Column chromatography
   b) Purification of tertiary mixture of amino acids by paper chromatography
   (Both experiments demonstration only)

2. Extraction of natural products such as Caffeine, Caesin.

3. Organic preparation: Any 4 preparations (involving two or more than two steps) involving the following representative reactions-
   1) Bromination
   2) Hydrolysis
   3) Nitration
   4) Condensation
5)Oxidation

4.Qualitativeanalysis – Separation of two component mixture and identification of components by chemical methods (about 4 – 5 mixtures)

5. Quantitative Analysis
   a) Estimation of ascorbic acid
   b) Estimation of glucose

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CO2	S	S	S	S	S	M	S	M	S	M	M	S	M	M	M	M
CO3	S	S	S	S	S	M	S	M	S	M	M	S	M	M	M	M
CO4	S	S	S	S	S	M	S	M	S	M	M	S	M	M	M	M

PCHE11 MEDICINAL CHEMISTRY AND DRUG DESIGN 5/5

Objectives:

1. To introduce the concept of molecular modeling and drug design.
2. To appreciate and understand the importance of bio-inorganic compound and bio-inorganic compounds in medicine
3. To understand the structure and mechanism of action of drugs.
4. To enable the students to apply the knowledge gained in the above concepts.

Course outcomes
On learning the course, the students will be able to .

1. Comprehend and apply the concept of molecular modeling
2. Perform quantum chemical calculations
3. Appreciate the importance of bio-organic compound and bio- inorganic compounds in medicine
4. Understand the structure and mechanism of action of drugs.

Unit I
Molecular modeling and Computer aided drug design.

Basic features of molecular modeling-Simulation for conformational analysis:Molecular mechanics, *Ab initio*, DFT and semi-empirical methods-Energy minimization; Local and global energy minima, saddle point-Electronic descriptors-Force fields-Monto Carlo simulation-QSAR-Regression methods-Function modules of molecular softwares.
Molecular docking- Molecular Dynamics; Introduction, basic principles, conformation analysis, Mechanics and dynamics of Bio-macromolecules.

Stages in drug development-conventional approach-Rational drug design-Target identification-Sequence to structure - Protein structure prediction - Homology modeling-Active sites-Lead structure identification, Target – Substrate Docking - Scoring-molecular descriptors - High throughout screening and combinatorial chemistry-Structure-activity relationship (SAR)–Toxicity, Patents

Unit II
Medicinal Bioinorganic Chemistry

Bioinorganic Chemistry of quintessentially toxic metals. Lead, Cadmium, Mercury, Aluminum, Chromium, Iron, Copper, Plutonium. Detoxification by metal chelation.Drugs that act by binding at the metal sites of Metalloenzymes.

Chemotherapy-Chemotherapy with compounds of certain non-essential elements. Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action - Lithium inPschycopharmocological drugs. Molecular channels and transport processes.

Unit III
Medicinal Bioorganic Chemistry

Introduction – Study of drugs – Important terminologies in pharmaceutical chemistry – Classification and nomenclature of drugs – Antibacterial drugs – Sulpha drugs: sulphanilamide,sulphadiazine –
Antibiotics: chloraphenicol, penicillin, Analgesics: morphine, heroin – Anticonvulsant: Barbiturates, oxazolindiones, streptomycin, terramycin

Unit IV

Vitamins : Vitamins A, B_1, B_2, C, E and H

Unit V
Drug Action

Mechanism of action of drugs – Metabolism of drugs – Absorption of drugs, Diabetes: control of diabetes, insulin – Cancer and antineoplastic drugs: antimetabolites, plant products – Cardio vascular drugs: Antiarrhythemic drugs, antihypertension drugs

Text Books

1. Andrew Leach, Molecular Modelling, Principles and Applications, 2nd Ed., Pearson, Prentice Hall, 1991.
2. G.L. Patrick, An Introduction to Medicinal Chemistry, Oxford University, Press, 2nd Ed., 2001.
3. A. R Leach, V. J. Gillet, An Introduction to Chemininformatics, Springer, The Netherlands, 2007.

Reference Books

1. J. Ghosh, Fundamental Concepts of Applied Chemistry, S. Chand and Co., New Delhi, 2006.
2. G. Thomas, Fundamentals of Medicinal Chemistry, John Wiley & Sons, 2003
3. A. Burger, Medicinal chemistry, I arts I and II, Wiley, N. Y.,1969.

Mapping of Cos with POs &PSOs:

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CO2	S	S	S	M	M	S	S	S	M	M	M	M	M	S	M	M
CO3	S	S	S	M	M	S	S	S	M	M	M	M	M	S	M	M
CO4	S	S	S	M	M	S	S	S	M	M	M	M	M	S	M	M

SEMESTER – II

PCHT21 ORGANIC CHEMISTRY – II 5/5

Objectives

1. To enable students to understand and appreciate the advanced concepts of stereochemistry and conformational analysis.
2. To provide knowledge and understanding of the various reagents in organic synthesis and important oxidation and reduction reactions.
3. To introduce the concept of asymmetric synthesis.
4. To enable students to apply the knowledge gained in the above concepts.

Course Outcomes
On learning the course, the students will be able to .

1. Evaluate the stability of various conformers of acyclic and cyclic systems using steric, electronic and stereoelectronic effects and correlate them to reactivity.
2. Use various models for determining stereoselectivity of various organic transformation
3. Understand and apply the various reagents in organic synthesis and design organic synthetic reactions.
4. Apply asymmetric transformations in a logical manner for the synthesis of chiral molecules.

Unit I

Conformational analysis of acyclic and cyclic system

Definition – restricted rotation about carbon – carbon single bonds – conformations of ethane and n-butane – conformational free energy – conformational isomers and atropisomers – population of conformers – influence of dipole – dipole repulsion, van der Waals attractive force, intramolecular H-bonding on the stability of conformers.

Conformational analysis of cyclohexane systems – stability and isomerism in mono and di substituted cyclohexane – flexible conformers – conformational analysis of cyclohexane and its derivatives, cyclohexanones – alkyl ketone effect - α - halocyclohexanones – anomeric effect, Decalins.

Unit II
Dynamic stereochemistry conformation and reactivity

Conformation and reactivity in acyclic systems – stereo electronic and steric factors – simple examples illustrating E2 and cis eliminations, intramolecular rearrangements and neighbouring group participation, Curtin-Hammett principle.WinsteinElliel Equation, Steric assisted and steric hindered reaction

Simple reactions illustrating stereo and stereoelectronic factors – esterfication, oxidation, nucleophilic substitution at ring carbons and elimination reactions - reactions involving intramolecular rearrangements – formation and cleavage of epoxides and neighbouring group participation – reactions of enols and enolates

Unit III
Reagents in organic synthesis

Use of the following reagents in organic synthesis and functional group transformation – Dicyclohexylcarbodiimide, 1,3 dithiane (reactive umpolung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and Prevost hydroxylation, DDQ Wilkinson's Catalyst – Wittig reaction

Unit IV

Oxidation and Reduction

Oxidation of organic compounds with reagents based on peroxides, peracids, ozone, oxides of osmium, chromium, iodine and selenium dioxide

Reduction of organic compounds with reagents based on $LiAlH_4$, $NaBH_4$, Raney Ni hydrazine, formic acid and dissolving metals. Clemmenson reaction, Wolf Kishner reduction, Birch Reduction.

Unit V Asymmetric Synthesis

Importance of asymmetric synthesis – problems with resolution methods – optical purity - enantiomeric excess – diastereomeric excess – chiral, substrate controlled, auxillary controlled, catalyst controlled and solvent controlled asymmetric synthesis, example for each case, synthesis of longifolene by EJ Corey method

Text Books

1. E.L.Eliel, Stereochemistry of Carbon Compounds, McGraw Hill, 1962.
2. V.M.Potapov, Stereochemistry, MIR Publishers, Moscow 1979.
3. D.Nasipuri, Stereochemistry of Organic compounds, 2nd Edn, New Age International, New Delhi, 1972.

Reference Books

4. E.L.Eliel , N.C.Allinger, S.J.Angyal and G.A.Morrision, Conformational analysis, Interscience, New York, 1965.
5. C.Djerassi, Optical Rotatory Dispersion – Application to Organic Chemistry, Mc Graw Hall, 1960.
6. R.E.Ireland, Organic Synthesis, Prentice Hall, 1969.
7. S.Turner, Design of Organic Synthesis, Elsevier, 1976.

8. S.Warren, Designing Organic Synthesis – A programmed introduction to synthon approach, Wiley, New York, 1978.
9. R.K.Makie, P.M.Smith, R.A.Aatkin, Guide book to Organic Synthesis, 2nd Edn., Longman Scientific and Technical, London, 1990.
10. C E Coates. M L H Green, P Powell K Wade Principles of Organometallic Compounds Chapman and Hall, 1977.
11. C E Coates. M L H Green, K Wade. Organometallic Compounds Vol I. Mathew, 1967.
12. J.M.Swan and D.St.C.Black, Organometallics in organic synthesis, Chapman and Hall, London, 1974.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
CO1	S	S	M	S	M	M	S	S	M	M	M	M	M	M	M	M
CO2	S	S	M	S	M	M	S	S	M	M	M	M	M	M	M	M
CO3	S	S	M	S	M	M	S	S	M	M	M	M	M	M	M	M
CO4	S	S	M	S	M	M	S	S	M	M	M	M	M	M	M	M

PCHT22 INORGANIC CHEMISTRY – II 5/5

Objectives:

1. To familiarize the bonding concepts and isomerism in coordination compounds.
2. To provide thorough understanding of the electronic spectra and reaction mechanisms of coordination compounds.
3. To enable the student understand and appreciate the structure and bonding in organometallic compounds and pi- acceptor complexes.
4. To enable the students to apply the knowledge gained in the above concepts.

Course Outcomes

On learning the course, the students will be able to

1. Identify the bonding, structure and reactivity of selected coordination complexes
2. Interpret their electronic spectra and magnetic properties.
3. Utilize the principles of transition metal coordination complexes in understanding functions of biological systems.
4. Understand the bonding , structure and applications of organometallic compounds

Unit I

Chemistry of Coordination Compounds

Brief review of the general characteristics of transition elements, nomenclature of coordination complexes, Isomerism in coordination compounds, types of ligands and chelate effect, stepwise and overall formation constants-determination of stability constant by Job's continuous variation method., VB theory and CFT - Splitting of d-orbitals under different geometries – CFSE – evidence for CFSE-factors affecting CFSE – spectrochemical series – Jahn-Teller distortion-application of d-orbital splittings to explain magnetic properties, spin, Limitations of CFT – MO theory – sigma – and pi-bonding in complexes – Nephelauxetic effect

Unit II
Electronic Spectra of Metal Complexes

Term symbols for atoms and ions – splitting of orbitals and terms in crystal fields – characteristics of d-d transitions – energy levels – Orgel and Tanabe – Sugano diagram – effect of Jahn – Teller distortion and spin-orbit coupling on absorption spectra – crystal field spectra of transition metal complexes – calculation of 10Dq and β for Co(II) (O_h and T_d) and Ni(II) (O_h) complexes- charge transfer spectra of bipyridine and related diimine systems

ORD and CD: Chirality and the special nomenclature of chiral coordination compounds - optical activity, ORD and CD – Cotton effect – absolute configurations of chiral coordination compounds

Unit III

Inorganic Reaction Mechanism

Electron transfer reactions: Outer-sphere and inner sphere electron transfer reactions – The Marcus theory – non-complementary reactions – synthesis of coordination compounds by electron transfer reactions.

Substitution reactions Trans Effect, substitution reactions of square planar complexes of Pt(II) and other d^8 metal complexes – significance of trans-effect – substitution reactions of octahedral complexes – acid and base hydrolysis reactions – anation reactions, the template effect and macrocyclic ligands.

Unit IV

Organometallics

The 18 electron rule – applications and limitations – Isolobal concept and its usefulness Hapticity, Metal alkyl and aryls – olefin and acetylene complexes – Zeise salt – Dewar-Chatt approach to bonding in olefins &cyclobutadiene complexes, cyclopentadiene and benzene complexes of transition metals (preparation, bonding and reactions), – Fluxional molecules. Homogeneous catalysis involving organometallics – oxidative addition and reductive elimination reactions – hydrogenation, isomerization and hydroformylation of olefins – carbonylation of methanol, oxidation of olefins (Wacker process) - heterogeneous catalysis – Ziegler-Natta polymerization of propylene.

Unit V
Pi-acceptor Complexes

Synthesis, structure and bonding of mono nuclear and poly-nuclear carbonyls – nitrosyl complexes – dinitrogen complexes – metal carbonylato complexes, carbonyl hydrides and complex metal cyanides.

Text Books

1. J.D. Lee, Concise Inorganic Chemistry, 5th Ed, Wiley, 1999.
2. J.E. Huheey, Inorganic Chemistry, 3rd. Ed., Harper & Row publisher, 1983
3. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, 3rd Ed, 1999

Reference Books

1. D.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed. 1994.
2. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4th Ed., John Wiley & Sons,1986
3. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Oxford University Press, 1996.
4. A.G. Sharpe, Inorganic Chemistry, Pearson Education, 2008.
5. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., ELBS, 1991.
6. F. Basolo, R.G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., John Wiley, 1967.
7. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.
8. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 1977.
9. Oxford Chemistry Primers Series, No.12, M. Bochmann,Organometallics 1: Complexes with transition metal-carbon σ bonds and No. 13
M. Bochmann,Organometallics 2: Complexes with transition metal- carbon π-bonds.
10. J.P. Collman, L.S. Hegedus, J.R. Nortan, R.G. Finke, Principles and Applications of Organotransition Metal Chemistry, University Science Books, 1980.
11. R. Hoffmann, Angew. Chem. Int. Ed., Engl. 21, 711-800, 1982.

Mapping of Cos with POs &PSOs:

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CO2	S	S	M	S	M	S	S	S	M	M	M	M	M	M	M	M
CO3	S	S	M	S	M	S	S	S	M	M	M	M	M	M	M	M
CO4	S	S	M	S	M	S	S	S	M	M	M	M	M	M	M	M

PCHT23 PHYSICAL CHEMISTRY – II 5/5

Objectives:

1. To provide a sound knowledge and understanding of the quantum chemical laws and their applications
2. To enable the students to understand and appreciate the importance of the reactions in surface and catalysis
3. To enable the students to appreciate the importance green chemistry and polymer chemistry
4. To enable the students to apply the knowledge gained in the above concepts.

Course Outcomes

On learning the course, the students will be able to

1. Solve the model problems in quantum mechanics and analyze the basis behind the postulatory method of quantum mechanics
2. Apply time independent perturbation theory to complex problems of molecular energy levels
3. Appreciate and apply the principles of green chemistry and polymer chemistry
4. Understand and appreciate the importance of the reactions in surface and catalysis

Unit I
Quantum Theory – I

Planck's quantum theory – Bohr atom model - Wave – Particle duality – Uncertainty Principle – Operators and commutation relations – Sums and product of operator, commutator, linear and non-linear operator, Hermitian and Hamiltonian operator, Postulates of quantum mechanics and Schrodinger equation – eigen functions and eigen value, - Free particle – Particle in a box – degeneracy-one and three-dimensional, distortion of the box and Jahn-Teller effect, quantum numbers, zero-point energy, orthogonalisation and normalityfinite potential barrier – tunneling.

Unit II
Quantum Theory – II

Derivation of angular momentum operator, Rigid rotator-Harmonic oscillator. The hydrogen atom – space quantization of electronic orbits – angular and radial part, electron spin - Approximate methods of solving the Schrodinger equation – The perturbation and variation methods – Application to He atom - Angular momentum– spin orbit interaction – vector model

of the atom – term symbols - Pauli exclusion principle Slater determinant. Atomic Structure Calculation

Unit III
Quantum Theory – III

Molecular Orbital and valence bond theory of molecules: The Born–Oppenheimer approximation, MO treatment of H_2^+, and MO and VB treatment of H_2 molecule – comparison of MO and VB methods. Bonding in homo and hetero nuclear diatomics
(HF, CO, NO) – polyatomic molecules concept of hybridization -Huckel theory of conjugated systems - application to ethylene, butadiene.

Unit IV
Surface Chemistry and Catalysis

Surface Phenomena: Physisorption and chemisorptions ,solid- liquid interfaces – contact angle and wetting, Adsorption from solution, , Gibbs adsorption isotherm — solid-gas interface — Freundlich, Langmuir, Temkin, BET isotherms – surface area determination.

Homogeneous catalysis – Acid-base catalysis – Acidity function – Enzyme catalysis – Michaelis–Menten kinetics.Kinetics of bimolecular surface reactions involving adsorbed species – Langmuir-Hinshelwood mechanism, Langmuir – Rideal mechanism – Rideal –Eley mechanism. Basic aspects of semiconductor catalysis and applications
Solar energy conversion – Photogalvanic cell – Photoelectrochemical cells – Electrolysis of water.

Unit V
Polymer Chemistry

Overview of polymers – Structure and classification of polymers – Degree of polymerization, Kinetics and mechanism of free radical and ionic polymerizations - Coordination polymerization, Zeigler–Natta catalysis Condensation – Self catalysed and Non-catalyzedpolycondensation, Copolymerization – Co-polymer - Equation and significance, Molecular weight of polymers– Determination of molecular weight – Light scattering and viscosity methods - Gel permeation chromatography.
Stereoregularity of polymers- significance of T_g and T_m

Text Books

1. A.K. Chandra, Introductory Quantum Chemistry, 4th Ed,. Tata McGraw Hill, 2009.
2. I.N. Levine, Quantum Chemistry, Allyn and Bacon, 1983
3. P.W. Atkins, Molecular Quantum Mechanics, 2nd Edn, Oxford Univ. Press, 1987
4. F.W. Billmeyer, Jr., A Text Book of Polymer Science, John Wiley, 1971.
5. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age Publishers, 1986.
6. P.W. Atkins,Physical Chemistry, 7th Ed., Oxford University press, 2002.
7. S. Glasstone, Text book of Physical Chemistry, McMillan, 1974.

Reference Books

1. D.A. McQuarrie, D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt. Ltd, 2003.
2. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1998.
3. F.L. Pillar Elementary Quantum Chemistry, McGraw Hill, 1968.
4. J.P. Lowe and K.A.Peterson, Quantum Chemistry, 3rd Edn., Elsevier 2006.
5. A.W. Adamson, Physical Chemistry of Surfaces, 4th Ed., John Wiley, 1982.
6. B.M.W. Trapnell, Chemisorption, Academic Press, 1955.
7. P.J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1971.
8. A. Tager, Physical Chemistry of Polymers, Mir Publishers, 1978.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO 7	PSO8	PSO 9	PSO 10
CO1	S	S	M	S	M	M	M	M	M	M	M	M	M	M	M	S
CO2	S	S	M	S	M	M	M	M	M	M	M	M	M	M	M	S
CO3	S	S	M	S	M	S	M	M	M	S	S	M	S	M	M	M
CO4	S	S	M	S	M	M	S	M	M	S	M	M	M	M	M	M

PCHP21 INORGANIC CHEMISTRY PRACTICALS 5/5

Objectives:

1. To develop skill identifying less common metal ions.
2. To develop skill in estimating metal ions through complexometric titrations.
3. To develop skill in estimating metal ions through redox titrations.
4. To develop skill in estimating metal ion through spectrophotometry.

Course Outcomes

On learning the course, the students will be able to

1. Identify less common metal ions.
2. Estimate metal ions through complexometric titrations.
3. Etimate metal ions through redox titrations.
4. Estimate metal ion through spectrophotometry

Practical – A : Qualitative Analysis

Less common metal ions – Mo, Se, Te, Ce, W, Ti, Zr, Th, U, V, Li (two metal ions in cationic and anionic forms)

Practical – B : Quantitative Analysis

a) EDTA titrations : Zn(II), Mg(II), Cu(II) and Ni(II)
b) Redox titrations : Fe(II) vs. Ce(IV) , Fe(II) vs. dichromate
NO_2^- vs. Ce(IV)
c) Spectrophotometric methods of analysis :
Fe(II) , Cu(II) .

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CO2	S	S	S	S	S	M	M	M	S	M	M	S	M	M	M	M
CO3	S	S	S	S	S	M	M	M	S	M	M	S	M	M	M	M
CO4	S	S	S	S	S	M	M	M	S	M	M	S	M	M	M	M

PCHE22 ANALYTICAL TECHNIQUES 5/5

Objectives:

1. To provide a sound knowledge and understanding of the various chromatographic techniques and their applications
2. To enable the students understand the different types of electroanalytical techniques.
3. To familiarize the students with spectrometric and thermal methods of analysis.
4. To enable the students to apply the knowledge gained in the above concepts.

Course Outcomes

On learning the course, the students will be able to

1. Apply various chromatographic techniques for separation and analysis of compounds
2. Understand and apply the different types of electroanalytical techniques
3. Apply AAS, XRD analytical techniques for compound identification and characterization.
4. Apply thermogravimetric techniques for characterization of compounds

UNIT I

Chromatography – I

HPLC: Introduction – Column Packing Materials – Solvent – Detectors – Recorder – Terms and Definitions used in HPLC analysis and applications.

Gas Chromatography: Introduction – Retention Time – Retention Volume – Efficiency – Career Gases – Preparation of Columns – Solid Supports – Stationary Phases Detectors – Temperature Effect – Quantitative and Qualitative analysis and applications.

UNIT – II

Chromatography – II

Gel Permeation Chromatography: (GPC)
Introduction – Types of gels – Selection of gels – Gel Preparation – Drying of gels – Packing of the Column Application of the sample – Resolution – Detectors and Applications.

Gas Chromatography Mass Spectrometry: (GCMS)
Introduction – Separators – Carrier gas – Sample Injection – Analyzer and Applications.

Liquid Chromatography Mass Spectrometry: (LCMS)
Introduction – Ionization – Belt Interface – Instrumentation and Applications.

Unit III

Electroanalytical methods

Amperometry-Principles and applications, amperometric titration with examples-comparison with other titration methods-Basic principles of electrogravimetry

Coulometry: principles- coulometry at controlled potential- coulometry at constant current-coulometric titrations-advantages and applications

Cyclic Voltammetry: Principles and simple analytical applications – Interpretation of cyclic voltammogram.

Unit IV

Spectrometry and thermal methods

Atomic absorption spectrophotometer(AAS)- principle, instrumentations and applications- types of interferences. Flame Emisssionspectroscopy (FES)- theory, instrumentationand applications, Difference between AAS and FES. Thermal methods of Analysis- principle, instrumentations and applications of TG, DTA and DSC-thermograms of calcium oxalate and $CuSO_4.5H_2O$

Unit V

Surface analysis and XRD

Photoelectron spectroscopy-theory-photo sources-electron analyzers - resolution-assignment of bands-Koopman'stheorm-principle, instrumentation and applications of UV, XPS and ESCA, Auger effect

Reference Books

1. D. C. Harris, Quantitative Chemical Analysis, 4th Ed., W. H. Freeman, 1995
2. G. D.Christian& J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn&Balon, 1986.
3. P.J. Wheatley, The Determination of Molecular Structure, (Unit V), Oxford University Press, 1968.
4. M.P. Seah, D. Briggs, Practical Surface Analysis by Auger and X-ray Photoelectron Spectroscopy, 2nd Ed., Wiley, 1992.
5. F.Moulder, W.F. Stickle, P.E.Sobol, K.D. Bomben, Handbook of X-ray Photoelectron Spectroscopy, Perkin-Elmer Corp., 1992.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
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CO2	S	S	S	S	S	M	M	M	S	M	M	M	M	M	M	M
CO3	S	S	S	S	S	M	M	M	S	M	M	M	M	M	M	M
CO4	S	S	S	S	S	M	M	M	S	M	M	M	M	M	M	M

SEMESTER – III

PCHT31 ORGANIC CHEMISTRY – III 5/5

Objectives:

1. To provide understanding of the basic concepts of photochemistry and various organic photochemical reactions.
2. To provide understanding of the pericyclic reactions.
3. To enable the student to analyze organic conpounds using various spectroscopic techniques.
4. To enable the students to apply the knowledge gained in the above concepts

Course Outcomes

1. Understand the basic concepts of photochemistry and various organic photochemical reactions
2. Understand pericyclic reactions
3. Apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.
4. Interpret the above spectroscopic data of unknown compounds.

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Unit I

Organic Photochemistry

Thermal versus photochemical reactions, basic concepts of organic photochemistry, Jablonski diagram – energy transfer mechanism – photochemical reactions of saturated ketones – Norrish type I and II reactions – photoreduction – Paterno - Buchi reaction – reaction of α, β unsaturated ketones – isomerisations – photochemistry of simple olefins – cis-trans isomerisation – di-π methane rearrangement – photochemical oxidations – oxidative coupling – photochemistry of arenes.

Unit II

Pericyclic reactions

Definition of pericyclic reactions – electrocyclic, cycloaddition and sigmatropic reactions – selection rules and stereochemistry for thermal and photochemical reactions – explanation on the basis of (i) FMO approach (Fukui), (ii) orbital correlation diagram approach (Woodward and Hoffmann) and (iii) aromatic transition state approach (Dewar and Zimmerman) Taking simple systems as example. Diels-Alder reaction, ene reaction, Sommelet – Hauser, Cope and Claisen rearrangements.

Unit III

Application of UV, IR and Mass Spectrometry in organic chemistry

UV spectra – types of excitation or transition probability – chromophores and auxochromes – factors affecting intensity and position of absorption bands – Dienes, Polyenes and Enones – Woodward Fischer rules.

IR Spectra – Hooke's law – factors affecting vibrational frequencies – characteristic group frequencies – Finger print region.

Mass spectrometry – basic principles – molecular ion peak, parent peak, fragments, metastable peak, isotope peaks – determination of molecular weight and molecular fragment – fragment pattern of simple organic molecules – Mclafforty rearrangement – Retero Diels Alder reaction.

Unit IV
Applications of NMR spectroscopy in organic structural determination

^{1}H NMR spectroscopy – origin of NMR spectra – chemical shift – number of signals – peak areas – multiplicity – geminal, vicinal and long range couplings – factors affecting chemical shifts and coupling constants, Karplus equation, AX,AX_3, AB_2, ACMX PATTERNSfirst order spectra, Simplification of complex spectra.

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^{13}C NMR spectroscopy: Broadband and Off resonance decoupling, comparison of ^{1}H and ^{13}C NMR – factors affecting intensity of signals – chemical shifts - γ - gauche effect

2D Techniques: ^{1}H-^{1}H COSY ,^{1}H-^{13}C COSY .

Unit V
Organic Synthesis

Importance of synthesis – carbon-carbon bond making reactions – functional group modifications – reterosynthetic analysis – synthons and synthetic equivalents – nucleophilic, electrophilic, electroneutral and free radical synthons – retron, partial retron and super retron - Chiron – umpolung – protection and deprotection – product, chemo, regio and stereoselectivities. One and two group disconnections – Diels Alder reactions – Robinson annulation method – 1,2- 1,3- 1,4- 1,5- and 1,6- difunctional compounds

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Reference Books

1. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds, 6th Ed., Wiley 1998.
2. J. Mohan, Organic Spectroscopy Principles and Applications, 2nd Ed., CRC, 2004.
3. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
4. D.L. Pavia, G.M. Lampman, G.S. Kriz,Introduction to Spectroscopy,3rd Ed., Brooks Cole, 2000.
5. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th Ed., Pearson, 1992.
6. J.D. Coyle, Organic Photochemistry, Wiley, 1985.
7. J.M. Coxon, B. Halton, Organic Photochemistry, 2nd Ed., Camb. Univ. Press, 1987.
8. G.R. Chatwal, Organic Phtochemistry, 1st Ed., Himalaya Publications house, 1998.
9. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, 1st Ed., Oxford University Press; 2000.
10. C.H.Depuy and D.L.Chapman, Molecular Reactions and Photochemistry, Prentice Hall, 1975.
11. T.L.Gilchrist and R.C.Storr, Organic Reactions and Orbital Symmetry, 2ndEdn., Cambridge, 1972.
12. R.E.Lehr and A.P.Marchand, Orbital Symmetry, A problem solving approach, Academic Press, New York, 1972.
13. A.L.Bellamy, An introduction to conservation of orbital symmetry, Longmann, 1975.
14. S.M.Muherjee and S.P.Singh, Pericyclic Reactions, Macmillan, 1976.

Mapping of Cos with POs &PSOs:

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CO2	S	S	S	S	S	M	M	M	S	M	M	M	M	M	M	M
CO3	S	S	S	S	S	M	M	M	S	M	M	M	M	M	M	M
CO4	S	S	S	S	S	M	M	M	S	M	M	M	M	M	M	M

PCHT32INORGANIC CHEMISTRY – III 5/5

Objectives:

1. To enable the students to analyze the inorganic compounds using various spectroscopic techniques.
2. To appreciate and understand the importance of nuclear reaction
3. To familiarize the important inorganic photochemical reactions.
4. To enable the students to apply the knowledge gained in the above concepts.

Course Outcomes

On learning the course, the students will be able to

1. Analyze inorganic compounds using various spectroscopic techniques.
2. Understand the principles and applications of nuclear reactions
3. Familiarize the important inorganic photochemical reactions.
4. Apply the knowledge gained in the above concepts.

Unit I

Infrared Spectroscopy

Spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO^-_4 – effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide

Unit II

NMR Spectroscopy

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^1H, ^{19}F, ^{31}P, ^{13}C) interpretation and applications to inorganic compounds- NMR spectra of P_4S_3,H_3PO_3,H_3PO_2 and HPF_2. ^{19}F NMR spectra of ClF_3, BrF_3 and equimolar mixture of TiF_6 and TiF_4 in ethanol – Effect of quadrupolar nuclei on the ^1H NMR spectra, Satellite spectra.

Systems with chemical exchange - study of fluxional behavior of molecules NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents.

Unit III

EPR Spectroscopy

Theory of EPR spectroscopy - Spin densities and McConnell relationship –presentation of the spectrum-hyperfine splitting, Applications of ESR to some simple systems such as CH_3, *p*-benzosemiquinone, Xe_2^+ - Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(III), Co(II), Ni(II) and Cu(II) complexes

Mossbauer Spectroscopy

Theory-Doppler effect - isomer shift-quadruple splitting-magnetic hyperfine splitting-application of MB spectroscopy to inorganic compounds

Unit IV

Nuclear Chemistry

Properties of nucleus – different types of nuclear forces – liquid drop model, shell model of nucleus – nuclear reactions induced by charged particles – Q value – nuclear reaction cross section, significance and determination – theory of nuclear fission – reactor and its components – production of feed materials for nuclear reactors – disposal of radioactive wastes – nuclear fusion, stellar energy. Application of radioisotopes in agriculture, industry and medicine – neutron activation analysis – hot atom chemistry.

Unit V

Inorganic Photochemistry

Elementary ideas on the photosystems I and II - Photochemistry of Cr(III), Co(III) and Ru(II) - coordination compounds – photoaquation – photoanation – photoisomerisation – photo redox reactions – charge transfer photo chemistry – photosensitization – solar energy conversiuon – photogalvanic cell – splitting of water to evolve hydrogen and oxygen – photochemistry of Pt(II) and Pt(IV) complexes.

Text Books

1. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern Company
2. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.
3. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd Ed., ELBS, 1987.
4. Arniger, Nuclear Chemistry

Reference books

1. R.S. Drago, Physical Methods in Chemistry, W. B. Saunders Company, 1992.
2. J. Lewis, R.G. Wilkins, Modern Coordination Chemistry, Inter Science publisher, 1960.
2. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.
3. Collected readings in Inorganic photochemistry, J. Chem. Edn. 1983.
4. G. J. Ferraudi, Inorganic photochemistry, 1973.
5. A.W. Adamson, E.D. Fleishcer, Concepts in Inorganic photochemistry, 1963.

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CO1	S	S	M	S	M	S	S	S	S	M	M	M	M	M	M	M
CO2	S	S	M	S	M	S	S	S	M	M	M	M	M	M	M	M
CO3	S	S	M	S	M	S	S	S	M	M	S	M	M	M	M	M
CO4	S	S	M	S	M	S	S	S	M	M	M	M	M	M	M	M

PCHT33PHYSICAL CHEMISTRY – III 5/5

Objectives:

1. To provide a sound knowledge and understanding of the concepts and applications of group theory.
2. To familiarize the theories behind various spectroscopic techniques
3. To provide knowledge and understanding of statistical thermodynamics and its applications.
4. To enable the students to apply the knowledge gained in the above concepts.

Course Outcomes

On learning the course, the students will be able to

1. Determine the symmetry operations of any small and medium-sized molecule and apply point group theory to the study of hybridization and spectroscopy.
2. Have a sound knowledge of the theories behind various spectroscopic techniques
3. Apply the concepts of statistical thermodynamics for the study of equilibrium reactions.
4. Understand to apply the concepts of statistical thermodynamics for the study of reaction rates.

Unit I
Group Theory: Concepts

Elements of symmetry – point group classification of molecules – definition and theorems of group – properties of group with examples - symmetry operations as elements of group – group multiplication table – similarity transformations – sub groups – classes – representation of groups - reducible and irreducible representations – Great orthogonality theorem (derivation and proof excluded) – character table for H_2O and NH_3 molecules – format and significance – direct products and simplified procedure for generating and factoring total representations. Symmetry adapted linear combinations – projection operators.

Unit II

Group theory : Applications

Molecular vibrations and their symmetry types in typical molecules – IR and Raman activity – bonding with central atom and formation of hybrid atomic orbitals in molecules such a BF_3, $(PtCl_4)_2CH_4$ – simplification of MO calculations – naphthalene, benzene – symmetries of molecular orbitals and electronic configurations – group theoretical selection rules – vanishing matrix elements selection rules for electronic transitions – electronic spectra of the carbonyl chromophore.

Unit III

Spectroscopy – I

General features of spectrum – Experimental techniques – Intensities of spectral lines and linewidths - Rotational spectra - Vibrational spectra – Rotation–Vibration spectra of diatomic and polyatomic molecules – Fermi resonance – Basic concepts of FTIR – Raman spectroscopy – Rotational Raman and vibrational Raman – Resonance Raman and Laser Raman – Electronic spectra of diatomic molecules – Franck-Condon principle – Vibrational and rotational fine structure – Fortrat diagram – Predissociation.

Unit IV

Spectroscopy – II

NMR – nuclear spins in a magnetic field – Zeeman effect – Larmor precession – Resonance phenomenon – Block equations – Spin - lattice and spin-spin relaxation times – Nuclear shielding and chemical shift – Spin-spin coupling – Basic principles of FT NMR – Inversion recovery and CPMG sequenced for T_1 and T_2 measurements – NMR instrumentaion.

ESR – Electronic zeeman effect – ESR spectrum of hydrogen atom (first order treatment) - g factors – Hyperfine constants – ESR of organic radicals in solution – McConnell's relation – ESR instrumentation.

Unit V
Statistical Thermodynamics

Thermodynamics probability and entropy – Maxwell-Boltzman, Bose-Einstein and Fermi- Dirac statistics and applications, - partition function and entropies for translatinl, rotational, vibrational and electronic motions of monoatomic and diatomic molecules – calculations of thermodynamic functions and equilibrium constants – specific heat of solids – Einstein and Debye theories.

Text Books

1. F.A. Cotton, Chemical Applications of group Theory, 3rd Ed., Wiley Eastern, 2004.
2. R.L. Carter, Molecular Symmetry and Group Theory John Wiley, 1998.
3. C.N. Banwell, E. McCash, Fundamentals of molecular Spectroscopy, 4th Ed., TMH, 2008.
4. B.P. Straughan, S.Walker Spectroscopy Vol.3, Chapman Hall, 1976.
5. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.
6. P.K. Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley, 1989.
7. P.W. Atkins, Physical Chemistry, 7th Ed., Oxford University press, 2002.

Reference Books

1. R.L. Flurry, Jr, Symmetry Groups – Prentice Hall, New Jersy 1980.
2. B.E. Douglas and C.A. Hollingsworth, Symmetry in Bonding and Spectra – An Introduction, Academic Press, 1985.
3. S.F.A. Kettle, Symmetry and Structure, John Wiley & Sons, 1985
4. D.A. McQuarrie, D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt. Ltd, 2003.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
CO1	S	S	M	S	M	M	M	M	M	M	M	M	M	M	M	S
CO2	S	S	M	S	M	M	M	M	S	M	M	M	M	M	M	S
CO3	S	S	M	S	M	M	M	M	M	S	M	M	M	M	M	S
CO4	S	S	M	S	M	M	M	M	M	S	M	M	M	M	M	S

PCHP33 PHYSICAL CHEMISTRY PRACTICALS 5/5

Objectives:

1. To develop skill in carrying out kinetics experiments
2. To develop skill in carrying out experiments related to distribution law and study phase diagrams.
3. To impart skill in analysis through conductometry.
4. To develop skill analysis through potentiometry

Course Outcomes

On learning the course, the students will be able to

- Explain the principle behind the experiments
- Plan and Perform experiments
- Interpret experimental results
- Perform estimation through conductometry and potentiometry

Any twenty experiments out of the following experiments (to be decided by the course teacher):

1. Kinetics – Acid Hydrolysis of Ester – Comparison of strength of acids.
2. Kinetics – Acid Hydrolysis of Ester – Determination of Energy of Activation (E_a).
3. Kinetics – Saponification of Ester – Determination of E_a by conductometry.
4. Kinetics – Persulphate – Iodide Reaction – Determination of order, effect of Ionic strength on rate constant.
5. Polymerization – Rate of polymerization of acrylamide.
6. Distribution Law – Study of iodine – Iodide equilibrium.
7. Distribution Law – Study of Association of Benzoic Acid in Benzene.
8. Study of phase diagram of two components forming simple eutectic.
9. Study of phase diagram of two components forming a compound.
10. Determination of molecular weight of substances by TT measurements.
11. Determination of Critical Solution Temperature of phenol water system and effect of impurity on SCT.
12. Adsorption – oxalic Acid\Acetic Acid on charcoal using Freundlich isotherm.
13. Conductometry – Acid – alkali titrations.
14. Conductometry – precipitation titrations.
15. Conductometry - Displacement titrations.
16. Conductometry – Determination of dissociation constant of weak acids.
17. Conductometry – Solubility product of sparingly soluble silver salts.
18. Verification of Onsager equation – conductivity method.
19. Determination of degree of hydrolysis and hydrolysis constant of a substance.
20. Potentiometric titrations – Acid alkali titrations.
21. Potentiometric titrations – Precipitation titration.
22. Potentiometric titrations – Redox Titrations.
23. Potentiometry – Determination of dissociation constant of week acids.
24. Potentiometry- Determination of solubility product and pKa

Reference Books

1. B.P. Levitt, Ed., Findlay`s practical Physical Chemistry, 9th Ed., Longman, 1985.
2. J.N. Gurtu, R. Kapoor, Advanced Experimental Chemistry, Vol.I, S.Chand& Co., 1987.
3. B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books,2009.

Mapping of Cos with POs &PSOs:

PO/PSO	PO 1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO 3	PS O4	PSO 5	PSO 6	PS O7	PS O8	PS O9	PS O10
CO1	S	S	S	S	M	M	M	M	S	M	M	S	M	M	S	M
CO2	S	S	S	S	M	M	M	M	S	M	M	S	M	M	S	M
CO3	S	S	S	S	M	M	M	M	S	M	M	S	M	M	S	M
CO4	S	S	S	S	M	M	M	M	S	M	M	S	M	M	S	M

PCHE33 Environmental Chemistry and Green Chemistry 5/5

Objectives:

1. To provide knowledge and understanding of the various types and ways to eradicate pollution.
2. To familiarize the various methods of water treatment.
3. To enable the students to appreciate the concepts of green chemistry.
4. To impart concern over the environment and insist to adopt eco-friendly methods

Course Outcomes

On learning the course, the students will be able to

1. Identify environmental problems related to pollution
2. Identify and utilize eco-friendly methods to protect environment
3. Understand and apply green chemical methods
4. Solve the problems related to environmental pollution

Unit I – Water Pollution

Types of water pollution,-Physical, chemical and biological types, ground water and surface water pollution – sources and harmful effects – sources and effects of major water pollutants –inorganic pollutants – oxygen demanding wastes - organic pollutants – plant nutrients – detergents – radioactive wastes – nuclear pollution – sources effects of ionizing and non-ionizing radiation. Significance of various water pollutants- thermal pollution

Unit II – Air Pollution

Atmosphere-structure – functions and photochemical reactions – sources of air pollution-natural and man made –acid rain, classification and effects of air pollutants – CO, CO_2, SO_2, SO_3,NO and NO_2 – hydrocarbon as pollutant – reactions of hydrocarbons and effects – particulate pollutants – sources and effects of Organic particulate and Inorganic particulate Green House effect – impact on global climate – role of CFC's – ozone holes – effects of ozone depletion – smog-components of photochemical smog-effects of photochemcial smog.

Unit III – Pesticides and Soil Pollution

Soil Pollution: Sources, Types, Pesticides – classification, mode of action – toxic effects of chlorinated hydro carbons, organophosphorous compounds and carbamates – alternatives to chemical pesticides – (pheromones, Juvenile harmones, chemosterilization)

Unit IV – Treatment of drinking water

Removal of suspended impurities, removal of micro-organisms, Treatment of Efflunets, 1º treatment,- Filteration, Coagulation, - 2º treatment –oxidation ponds- 3º treatment-reverse osmosis, electrodialysis- Nanofilteration.
Treatment of water for Industrial purpose- Hardness-softening methods-Zeolite-Limo-soda-Ion Exchange methods.

Unit V Green Chemistry

Green Chemistry - Definition, principles and requirements, water mediated reactions - solventless reactions – microwave assisted reactions – solid supported reactions – uses of ionic liquids and supercritical carbondioxide reaction in organized media – uses of calixarene, zeolites, cyclodextrin and other supramolecules as media for selection reactions - clay catalysed reactions – definitions and examples of multicomponents reaction and tandem reactions – atom economy reactions.

Text Books

1. AsimK.Das, Environmental Chemistry with Green Chemistry, Books & Allied (P) Ltd, Kolkata, 2012.
2. B.K.Sharma, Environmental Chemistry, Goel Publishers, 2001.

Reference books

1. A.K. De, Environmental Chemistry, New Age International, Fifth Edition, 2005.
2. C. J. Gonzalez, D. J. C. Constable, Green Chemistry and Engineering, A practical Design approach, Wiley Interscience, 2011
3. S. Parsons, B. Jefferson, Introduction to potable water treatment processes, Wiley – Blackwell, 2006.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
CO1	S	M	M	M	M	S	M	M	M	M	S	M	M	M	M	M
CO2	S	M	M	M	M	S	M	M	M	M	S	M	M	M	M	M
CO3	S	M	M	M	M	S	M	M	M	M	S	M	M	M	M	M
CO4	S	M	M	M	M	S	M	M	M	M	S	M	M	M	M	M

SEMESTER – IV

PCHT41 Chemistry of Natural products and Bioinorganic chemistry 5/5

1. To enable the students to understand the structure of organic natural products.
2. To provide knowledge of the structures of metalloproteins and metalloenzymes.
3. To familiarize the importance of natural product and bio-inorganic compounds.
4. To enable the students to know and appreciate the importance of chemistry of nature.

Course Outcomes

On learning the course, the students will be able to

1. Understand the structure of organic natural products.
2. Identify the structures of metalloproteins and metalloenzymes.
3. Appreciate the importance of natural products and bio-inorganic compounds.
4. Know and appreciate the importance of chemistry of nature.

Unit I

Proteins, peptides, Nucleic acid, Fats and Lipids

Structure and properties of amino acids and proteins, Zwitterions and purification of proteins
Nucleic acids – nucleotides and nucleosides – structure of purine and pyrimidine bases; Phosphordiester bond, double helical structure of DNA. Structure of RNA (tRNA)
Fatty acids - structure and classification, lipids classification and function (Simple, compound and derived lipids)

Unit II

Terpenoids

Classification of terpenoids with examples – isoprene rules – General methods of structural determination of terpenes – structure and synthesis of *alpha*-pinene, cadinene, zingeberene and abietic acid

Unit III

Alkaloids

General methods of structure analysis of alkaloids – Hoffmann, Emde and von Braun degradations – Structure and synthesis of quinine, papavarine, atropine, narcotine, reserpine and lysergic acid.

Unit IV

Steroids

Types of steroids – structure, stereochemistry and synthesis of cholesterol – Structural features of bile acids – Sex harmones – androsterone, testerosterone, estrone, estriol, estradiol, progesterone - Structure of ergosterol.

Circular birefringence, optical rotary dispersion, circular dichroism – Cotton effect curves – octant rule – axial haloketone rule - Applications of chiroptical properties in configurational assignments.

Unit V

Bioinorganic Chemistry

Metal ions in biological systems: heme proteins, hemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferrin, cytochromes and vitamin B12; Iron-sulphur proteins: rubredoxin, ferredoxin and model systems. Classification of copper proteins and examples - Electron transfer (Cu, Zn) – Blue copper proteins

Metalloenzymes: active sites, carboxy peptidase, carbonic anhydrase, superoxide dimutase, xanthine oxidase, peroxidase and catalase; photosynthesis, water oxidation, nitrogen fixation, nitrogenase; ion pump, metallodrugs.

Text Books

1. I.L. Finar, Organic Chemistry, Vol.II, ELBS 1985
2. S.J. Lippard, J.M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, 1977.
3. Gurdeep R Chatwal,Organic Chemistry Of Natural Products, Volume I , Himalaya Publishing House, 2009
4. L. Stryer, Biochemistry, 4th Ed., W. L. Freeman and Co, New York, 1995.
5. D. L. Nelson, M. M. Cox, Lehninger Principles of Biochemistry, 5th Ed.

Reference Books

1. W. Kaim, B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, 1994.
2. Bioinorganic Chemistry, Chem. Education, 62, No. 11, 1985.
3. G.L. Eichorn, Inorganic Biochemistry, Volumes 1 & 2, 2nd Ed., Elsevier, 1973.
4. J.N.Davidson, The Biochemistry of Nucleic acids, ELBS, 1965.
5. J.L.Simonsen, The Terpenes, Vols 1-4, Academic Press, N.Y. , 1957.
6. K.Nakanishi, Natual Products Chemistry, Vols. I & II, Academic Press, 1975.
7. W.Klyne, The Chemistry of Steriods, Methuen and co., N.Y. 1965.
8. Androsterone and Testosterone: *J. Chem. Soc. Perkin Trans. I*, **1986**, 117-123.
9. Estrone, Estradiol and 2-Methoxyestradiol:*J. Org. Chem.***2009**, *74*, 6362-6364.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
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CO2	S	M	M	M	M	S	S	S	M	M	M	M	M	S	M	M
CO3	S	M	M	M	M	S	S	S	M	M	M	M	M	S	M	M
CO4	S	M	M	M	M	S	S	S	M	M	M	M	M	S	M	M

PCHT42 NANOCHEMISTRY AND SUPRAMOLECULAR CHEMISTRY 5/5

Objectives

1. To enable students to understand and appreciate the importance of Nanoscience and Technology.
2. To impart knowledge in the synthesis and applications of Nanomaterials.
3. To provide knowledge and understanding of the concepts of Supramolecular chemistry
4. To enable the students to apply the knowledge gained in the above concepts.

On learning the course the students will be able to

1. Appreciate the importance of Nanoscience and Technology.
2. Familarize the synthetic techniques and applications of Nanomaterials.
3. Comprehend the concept of Supramolecular chemistry and its applications
4. Apply the knowledge gained in the above concepts.

Unit I: Nanoscience and Nanotechnology

Definition of nanodimensional materials, Classification of Nanomaterials – Significance of surface to volume ratio, Size effects - Importance of Nanomaterials - - Simple examples of unique properties of nanosized materials - Elementary aspects of bionanotechnology - Some important recent discoveries in nanoscience and technology, Applications of Nanomaterials

Unit II: Carbon-based Nanomaterials

Carbon: Bonding in Carbon compounds, Discovery of Cubane, Fullerenes: synthesis, chemical reactions and properties, Carbon Nanotubes: Structure of Single-Walled Carbon nanotubes, physical properties of Single-Walled Carbon nanotubes, synthesis of Carbon nanotubes, growth mechanisms, chemical modification of Carbon nanotubes –DiamondoidNanomaterials: diamondoids, thin diamond films (and other ultrahard substances) – Chemical modification of CVD Diamond

Unit III: Growth techniques and Characterization tools of nanomaterials

Introduction – top-down vs bottom-up technique – Lithographic process and its limitations – Nonlithographic techniques : Sputtering, Chemical Vapour Deposition, Pulsed Laser Deposition, Sol-Gel technique-nucleation and growth processes, Electrodeposition, Scanning Probe Microscopy – General Concept and defining Characteristics of AFM – Electron Microscopy – Transmission Electron Microscopy

Unit IV: Supramolecular Chemistry – I

Introduction to Supramolecular Chemistry – definitions – concepts – molecular forces - covalent bonding, ion – ion, ion – dipole, dipole – dipole, hydrogen bonding, cation – π, π-π interactions, van der Waals forces, hydrophobic and solvent effects – Common motifs in Supramolecular Chemistry – Host/Guest Chemistry, cation, anion and neutral molecule binding. Molecular receptors and design principles.

UNIT V: Supramolecular Chemistry – II

Principles of molecular association and organization – SAMs, micelles, vesicles and cell membrane –Molecular channels and transport processes - Supramolecular reactivity and catalysis- Molecular devices and Nanotechnology

Text books

1. T. Pradeep, NANO: The Essentials: Understanding Nanoscience and Nanotechnology, McGraw Hill Education; 1 edition, 2017)
2. B. S. Murthy, P. Shankar, B. Raj, B. B. Rath, and J.Murday,Textbook of Nanosciene and Nanotechnology, University Press India Private Limited, I edition, 2012.

Reference Books

1. G.L.Hornyak, J.Dutta, H.F.Tibbals, A.K.Rao, Introduction to Nanoscience, CRC Press, 2008.
2. Mich Wilson, KamaliKanengara, Geoff smith, Michelle Simmons and BurkherdRaguk, Nanotechnology Basic Science and Energy Technologies, Overseas press (I), N.D. 2005
3. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, ao 2, Wiley – VCH, Weinheim, 2004.
4. J. W. Steed, J. L. Atwood, "Supramolecular Chemistry", Wiley, 2000.
5. Supramolecular Chemistry: Concepts and Perspectives by Jean-Marie Lehn, VCH, 1995.
6. A Practical Guide to Supramolecular Chemistry by Peter Cragg, Wiley, 2005.
7. Supramolecular Chemistry - Fundamentals and Applications: Advanced Textbook by Katsuhiko Ariga and ToyokiKunitake, Springer, 2006.
8. Core Concepts in Supramolecular Chemistry and Nanochemistryby Jonathan W. Steed, David R. Turner, and KarlWallaceWiley, 2007.
9. Supramolecular Chemistry (Oxford Chemistry Primers, 74) by Paul D. Beer, Philip A. Gale, and David K. Smith, Oxford Science Publications,1999.

Mapping of Cos with POs &PSOs:

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CO1	S	M	M	M	M	S	M	S	M	M	M	M	M	M	M	M
CO2	S	M	S	S	M	S	M	S	S	M	M	M	M	M	M	M
CO3	S	M	M	M	M	S	M	M	M	M	M	M	S	M	M	M
CO4	S	M	M	M	M	S	M	M	M	M	M	M	S	M	M	M

PCHP43 Project Work

Course Outcomes

On learning the course, the students will be able to

1. Analyze the existing problems for which research can provide solutions and Select the problem for research
2. Know the various chemical publishers, journals and perform literature survey
3. Synthesize new chemical compounds through various methods
4. Characterize the compounds using various analytical and spectroscopical studies.

Mapping of Cos with POs &PSOs:

PO/PSO	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO7	PSO8	PSO9	PSO10
CO1	S	S	S	S	S	S	S	S	S	M	M	S	M	M	M	M
CO2	S	S	S	S	S	S	S	S	S	M	M	S	M	M	M	M
CO3	S	S	S	S	S	S	S	S	S	M	M	S	M	M	M	M
CO4	S	S	S	S	S	S	S	S	S	M	M	S	M	M	M	M