

404 - M.Sc. CHEMISTRY

Programme Structure and Scheme of Examination (under CBCS) (Applicable to the candidates admitted from the academic year 2022 -2023 onwards)

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Cours	Study Components & CourseTitle	Hours/W	Credit	VI	ESE	Total
	SEMESTER – I					
22PCHEC11	Core Course– I: Organic Chemistry -I	4	3	25	75	100
22PCHEC12	Core Course – II: Inorganic Chemistry -I	4	3	25	75	100
22PCHEC13	Core Course- III: Physical Chemistry - I	4	3	25	75	100
22PCHEP14	Core Practical – I: Organic Chemistry Practical - I	6	3	40	60	100
22PCHEP15	Core Practical – II: Physical Chemistry Practical -I	5	3	40	60	100
22PCHEE16	Core Elective – I	4	3	25	75	100
22PCHEO17	Open Elective – I	3	3	25	75	100
	Total	30	21			700
	SEMESTER – II					
22PCHEC21	Core Course-IV: Organic Chemistry -II	4	3	25	75	100
22PCHEC22	Core Course- V: Inorganic Chemistry -II	4	3	25	75	100
22PCHEC23	Core Course- VI: Physical Chemistry - II	4	3	25	75	100
22PCHEP24	Core Practical – III: Organic Chemistry Practical - II	6	3	40	60	100
22PCHEP25	Core Practical – IV: Inorganic Chemistry Practical -I	6	3	40	60	100
22PCHEE26	Core Elective – II	4	3	25	75	100
22PHUMR27	Compulsory Course: Human Rights	2	2	25	75	100
	Total	30	20			700

List of Core Electives (Choose 1 out of 3 in each Semester)

Semester	Course Code	Course Title	H/W	С	CIA	ESE	Total
	22PCHEE16-1	Polymer Chemistry	4	3	25	75	100
Ι	22PCHEE16-2	Materials Chemistry	4	3	25	75	100
	22PCHEE16-3	Pharmaceutical Chemistry	4	3	25	75	100
	22PCHEE26-1	Green Chemistry	4	3	25	75	100
II	22PCHEE26-2	Supra Molecular Chemistry	4	3	25	75	100
	22PCHEE26-3	Nano Chemistry	4	3	25	75	100

List of Open Electives (Choose 1 out of 3 in each Semester)

Semester	Course Code	Course Title	H/W	С	CIA	ESE	Total
	22PCHEO17-1	Food Chemistry	3	3	25	75	100
Ι	22PCHEO17-2	Industrial Chemistry	3	3	25	75	100
	22PCHEO17-3	Medicinal Chemistry	3	3	25	75	100

SEMESTER: I		CREDIT:3
CORE – I	ZZPCHECTT: ORGANIC CHEMISTRY -I	HOURS:60

- 1) To learn the basic aspects of stereochemistry
- 2) To gain knowledge about the reactive intermediate and reactions involving free radicals
- 3) To study the mechanisms of Aliphatic Nucleophilic and electrophilic substitutions
- 4) To learn the concepts of Aromaticity, Anti aromaticity and Homo aromaticity of Benzenoid and Non- benzenoid compounds
- 5) To accrue skill of predicting the mechanisms of Aromatic substitution reactions.

UNIT I: Stereochemistry – I

Optical isomerism - chirality - asymmetry and dissymmetry - enantiotopic and diastereotopic ligands and faces. R, S- notations of molecules with one and two asymmetric centers. Inter conversion of Sawhorse, Newman and Fischer projections. Erythro and threo nomenclature, E and Z nomenclature. Absolute configurations of chiral biphenyls, allenes and spiranes. Asymmetric synthesis - Cram's rule and Felkin- Ahn Modification. Stereospecific and stereoselective reactions.

UNIT II: Reactive intermediates and reactions involving free radicals 12 hrs

Structure, reactivity, formation, stability and reactions involving carbocations, carbanions, free radicals, carbenes and nitrenes. Long and short-lived free radicals - methods of generation of free radicals - detection of free radicals by ESR - Addition of free radicals to olefinic double bonds – aromatic radical substitutions reactions - decomposition of diazo compounds – phenol coupling - Sandmeyer reaction - Gomberg reaction - Pschorr reaction - Ulmann reaction and Hunsdiecker reaction.

UNIT III: Aliphatic Nucleophilic and Electrophilic Substitutions

12 hrs

Substitution at saturated reaction center (carbon). $SN1,SN2,SN_i$ mechanisms – Reactivity, structural and solvent effects. Neighbouring group participation – substitution in Norbornyl and bridgehead systems – Substitution at carbon doubly bonded to oxygen. Alkylation and acylation of active methylene compounds, hydrolysis of esters. SE_1 , SE_2 , SE_i mechanisms – reactivity. halogenation of aldehydes and ketones and decarboxylation of aliphatic acids, Hell-Volhard-Zelinsky reaction, Stork – enamine reaction.

3

UNIT IV: Aromaticity

Aromaticity of benzenoid - non-benzenoid, and heterocyclic compounds -Huckel's rule -Aromatic systems with π electron numbers other than six - nonaromatic (cyclooctatetraene etc.) and anti-aromatic system (cyclobutadiene etc.) system with more than 10π electrons - Annulenes upto C18 (synthesis of all these compounds is not expected).

UNIT V: Aromatic substitution reactions

12hrs

12hrs

Electrophilic substitution reactions: The arenium ion mechanism – Orientation and reactivity – typical reactions – nitration, halogenation, alkylation, acylation and diazonium coupling. Reimer- Tiemann, Vilsmeyer- Hack, Gattermann, Kolbe reactions. Electrophilic substitution of furan, pyrrole, thiophene and pyridine- Noxide. Nucleophilic substitution reactions: Aromatic Nucleophilic Substitution by SN1 mechanism through Meisenheimer complex and by Elimination - Addition mechanism. Methods of generation and reactions of aryne intermediate. Aromatic nucleophilic substitution of activated aryl halides, Ziegler alkylation and Chichibabin reaction.

COURSE OUTCOMES

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

- 1) Describe the concept of Stereochemistry
- 2) Compare the stabilities of various reactive intermediates.
- 3) Analyse and propose reasonable mechanism for Substitutions in Aliphatic molecules
- 4) Compare the stabilities of molecules based on aromaticity
- 5) Analyze the mechanisms of Aromatic Substitution reactions

Text Books

- 1) Eliel. E. N. (2008). Stereochemistry of Carbon Compounds, Tata McGraw Hill Ed, Reprint, Noida (UP).
- 2) Nasipuri. D. (2005). Stereochemistry of Organic Compounds, New Age International (P) Ltd, New Delhi.
- Kalsi, P. S. (1993). Stereochemistry, Conformation analysis and Mechanism (2nd Edition), Chennai: Wiley Eastern Limited.
- Clayden, J., Greeves, N., & Warren, S. (2012). Organic Chemistry (2nd Ed.). UK: Oxford University Press.
- Norman, R. O. C. & Coxon, J. M. (2003). Principles of Organic Synthesis (3rd Ed.). London (UK): Chapman & Hall.
- Smith, M. B. (2016). March's Advanced Organic Chemistry (7th Ed.). New York: John Wiley & Sons.
- 7) Carey, F. & Sundberg, R. J. (2007). Advanced Organic Chemistry (5th Ed., Part A and B.). Berlin: Springer Science + Business Media.

Supplementary Reading

- 1) Graham Solomons, T.W. Craig, B. Fryhle. (2011). Organic chemistry (10th edition.). John Wiley & Sons, Inc.
- 2) Pine, S. H. (1987). *Organic chemistry* (5th edition.). New York: McGraw Hill international edition chemistry series.
- 3) Seyhan, N. Ege. (1998). Organic chemistry structure and reactivity (3rd edition.). New Delhi: A.I.T.B.S.
- 4) Kalsi, P. S. (2007). Organic Reactions: Stereochemistry and Mechanism through solved problems (4th Ed.). New Delhi: New Age International (P) Ltd.

	PO1	PO2	PO3	PO4	PO5		
CO1	3	2	3	3	2		
CO2	2	2	3	3	3		
CO3	3	2	2	3	3		
CO4	2	3	3	3	3		
CO5	2	2	3	3	2		

SEMESTER: I 22PCHEC12: INORGANIC CHEMISTRY - I CORE – II

COURSE OBJECTIVES

- 1) To know about the structure and bonding of inorganic compounds and the inorganic polymers.
- 2) To study the concept of coordination chemistry and stability of the complexes
- 3) To gain knowledge of metal-ligand orbital overlap, molecular orbital theory and energy level diagrams etc.,
- 4) To learn about the mechanism of substitution reactions of octahedral complexes.
- 5) To acquire skill of using substitution reactions of square planar complexes and electron transfer reactions for complexes.

UNIT I: Polymeric Inorganic Compounds

Chains: Isopolyacids and heteropolyacids – Structure and bonding of isopoly and 6- and 12 Heteropolyanions. Rings: Phosphazenes, Linear and Cyclic phosphazenes, Phosphazene Polymers. Polymers: Silicates - Structure and Properties - Correlation - Distinction between 2D and 3D silicates, Zeolite types and examples, Shape selectivity in zeolites, Silicones and their applications. Cages: Structures and classification of higher boranes, carboranes, metallocarboranes -Wade's rule - Stylx number. Clusters: Metal Clusters - Dinuclear, Tetranuclear and hexanuclear clusters - Cubane clusters and Zintl Clusters.

NIT II: Coordination Chemistry-I

Stability of complexes, thermodynamic aspects of complex formation, factors affecting stability, HSAB approach. Determination of stability constants by spectrophotometric, polarographic and potentiomteric methods. Stereochemical aspects, stereoisomerism in inorganic complexes, isomerism arising out of ligand distribution and ligand conformation, chirality and nomenclature of chiral complexes, optical rotatory dispersion and circular dichroism. Macrocyclic ligands, types, porphyrins, corrins, Schiff bases, crown ethers and cryptates.

UNIT III: Coordination Chemistry – II

Evidences for metal-ligand orbital overlap, molecular orbital theory and energy level diagrams, concept of weak and strong field ligands, Jahn-Teller distortion, charge - transfer spectra. Russell-Sander's coupling - L-S coupling and micro states – Ground state terms for $d^1 - d^{10}$ ions – Derivation of terms for p^2 , p^3 , d^1 and d² configurations – Hund's rules in the determination of lowest energy states – Selection rules for electronic transitions - charge transfer transitions - d-d transitions, Orgel and Tanabe - Sugano diagrams, nephelauxetic effect, spectral and magnetic characteristics of transition metal complexes.

12 hrs

12 hrs

Unit – IV: Reaction Mechanism – I

Substitution reactions of octahedral complexes: Labilities, inertness, stability and instability of coordination compounds- Nature of substitution reactions-Theoretical approach to substitution mechanisms-Mechanism of substitution reactions of complexes of cobalt-acid hydrolysis-base hydrolysis of cobalt (III) complexes. Racemisation and isomerisation: Twist mechanisms for isomerisation – Intramolecular mechanisms for racemisation.

Unit – V: Reaction Mechanism – II

12 hrs

Substitution reactions of square planar complexes: Reactions of Pt (II) complexes- Trans effect- Theories of trans effect-Mechanism of substitution-kinetics of Pt (II) complexes. Electron transfer reactions-Electron Tunneling hypothesis-Marcus-Hush theory. Atoms transfer reaction-one electron and two electron transfer-inner sphere and outer sphere mechanism.

COURSE OUTCOMES

The student will be able to

1) Gain knowledge about the structure and bonding of Inorganic compounds and explain Isopolyacids and hetropolyacids of Vanadium, Chromium, Molybdenum and Tungsten.

2) Illustrates the chemistry of metal clusters and discuss polyhedral boranes, carboranes and metallocarboranes

3) Explain the stability constant of co-ordination complexes and stereo chemistry for co-ordination complexes

4) Apply the molecular orbital theory and energy level diagrams, concept of weak and strong field ligands, Jahn-Teller distortion etc.,

5) Illustrate the Substitution reactions of square planar complexes and electron transfer reactions

Text Books

- 1) Huheey, J. E. (1993). Inorganic Chemistry (IV Edition.). NY: Harper and Collins.
- 2) Purcell, K. F. & Kotz, J. C. (1977). Inorganic Chemistry. USA: WB Saunders Co.
- 3) Gopalan, R. (2001). *Concise Coordination Chemistry*. Vikas Publishing House.
- 4) Lee, J. D. (1991). Concise Inorganic Chemistry. US: Springer
- Das, A. K (2016). Fundamental Concepts of Inorganic Chemistry (2nd editon., Vol 1, 2 & 3). CBS publisher and Distribution Pvt. Ltd.
- 6) Manku, G.S. (1994) *Theoretical Principles of Inorganic Chemistry*. New Delhi: Tata McGraw Hill Publishing Company Ltd.
- 7) Ray, N. H. Inorganic Polymers. Academic Press.

Supplementary Readings

- 1) Cotton, F. A. & Wilkinson, G.W. (1988). Advanced Inorganic Chemistry A comprehensive Text. John Wiley & Sons
- 2) Shrivers, M. C., Atkins, P.W & Langford, CH. (1990). Inorganic Chemistry. Oxford University Press.
- 3) Greenwood, N. N. & Earnshaw. (1984). Chemistry of the Elements. New York: Pergamon Press,
- 4) Kettle, S. F. A. (1973). Coordination Chemistry. ELBS.
- 5) Dogulas, B. E., McDaniel, D. H., & Alexander J. J. (1983). Concepts and Models of Inorganic Chemistry. Oxford IBH.
- 6) Figgis, B. N. (1966). Introduction to Ligand Fields. Interscience.
- 7) Mutterties, E.L. (1975). Polyhedral Boranes. New York: Academic Press.
- 8) Day, M.C. & Selbin, J. (1974). Theoretical Inorganic Chemistry. New York: Van Nostrand Co.
- 9) Mingos, D. M. P. & Wales, D. J. Introduction to Cluster Chemistry. Prentice Hall.

PO1 PO2 PO3 PO4 PO5 CO1 3 2 3 2 3 2 3 CO2 2 2 3 CO3 3 2 3 3 2 2 2 CO4 3 2 3 CO5 2 3 3 2 2

SEMESTER: I		CREDIT:3
CORE – III	22PCHEC13: PHYSICAL CHEMISTRY -I	HOURS:60

- 1) To understand the theories of chemical kinetics in reaction mechanisms.
- 2) To apply the kinetic concepts in homogenous and heterogeneous catalyzed reactions.
- 3) To study about Surface Chemistry, surface tension and catalysis.
- 4) To identify the symmetry of elements, symmetry operations and apply the fundamentals of group theory in electronic spectroscopy
- 5) To appreciate the principals involved in the Rotational and vibrational spectroscopic techniques.

UNIT I: Chemical Kinetics – I

Theories of reaction rates and factors influencing the reaction rate: ARRT (Eyring's theory), Thermodynamic derivation of ARRT-comparison of ARRT with collision theory (A , $\Delta S^{\#}$, E_a and $\Delta H^{\#}$) – kinetic isotope effects, Marcus electron transfer theory-inner and outer electron transfer. Theory of unimolecular reactions-Lindemann's theory – Steady State approximation-chain reactions-photochemical reaction between hydrogen and halogens (Cl₂ and Br₂) – gas phase auto-oxidations, explosions-hydrogen-oxygen reaction.

UNIT II: Chemical Kinetics – II

12 hrs

12 hrs

Application of ARRT to solution kinetics-effects of solvents, double sphere model, effect of ionic strength on ionic reactions – influence of pressure on reaction rates in solution-significance of volume of activation-substituent effects – Hammett and Taft equations. Homogeneous catalysis, acid-base catalysis – types and mechanism, derivation of rate law for protolytic acid catalysis and explanation for Arrhenius and van't Hoff intermediates, Bronsted relations- Hammett-Deyrup acidity function – enzyme catalysis-mechanism of single substrate reaction-Michaelis-Menton equation - Influence of pH, concentration and temperature, Line Waver plot and Eddi – Hofstee plot. Fast reactions-study of kinetics by stopped flow technique, relaxation methods, T and P- jump methods, flash photolysis and magnetic resonance method.

UNIT III: Surface Chemistry

Adsorption-physisorption and chemisorptions – Langumuir, BET & Gibbs adsorption isotherms- surface area determination – Heat of adsorption, determination. Adsorption from solutions - surface films. Surface tension – effect of electrolytes, non-electrolytes and surface-active agents –micelles and reverse micelles. Solublisation, micro emulsions Heterogeneous catalysis – semiconductor catalysis, n-and p-type surfaces – kinetics of surface reactions involving adsorbed species – Langmuir - Hinshelwood mechanism. Langmuir – Rideal mechanism and Rideal - Eley mechanisms.

UNIT IV: Group Theory

Group theory -symmetry of elements and symmetry of operations, point groups of molecules, properties of a group and sub-group, isomorphism, cyclic, abelian, class- similarity transformation and conjugate, matrix representation – product of symmetry operations, group multiplication tables (C_n , C_{nv} and D_{nh} only) great orthogonality theorem and its consequences, construction of character tables (C_{2v} and C_{3v}). Direct products– reducible and irreducible representation – Wave function as bases for irreducible representation. Transition moment integral – spectroscopic selection rules to IR, Raman (H_2O , NH_3 , trans- N_2F_2) and electronic spectroscopy (HCHO). Hybridization schemes of orbitals – (sp, sp² and sp³ for ethylene and butadiene.

UNIT-V: Rotational and Vibrational Spectroscopy

12 hrs

Basic aspects of Spectroscopy-characterization of electromagnetic radiation, quantization of energy. Microwave Spectroscopy-Rotation of molecules and selection rules, Diatomic molecules; Rigid and non-rigid rotator, Rotational constant and centrifugal distortion. Techniques and instrumentation. Vibrational spectroscopy-diatomic molecules, Harmonic and a harmonic oscillator, zero-point energy - force constant -fundamental absorption and overtones (hot bands, fermi resonance)- polyatomic molecules-techniques and instrumentation of FTIR.

COURSE OUTCOMES

At the completion of this course, the students will be able to

- 1) derive the rate equation from mechanistic data and calculation
- 2) relate microscopic properties of molecules with macroscopic thermodynamic observables
- 3) gain knowledge about the Surface Chemistry and its mechanisms.
- 4) apply group theory for molecules like water, ethylene, butadiene etc...
- 5) imbibe basic aspects of spectroscopy and apply to poly atomic molecule

Text Books

- 1) Philip Mathews. (2003). Advanced Physical Chemistry. New Delhi: Foundation Books.
- 2) Puri, R., Sharma, L.R., & Pathania, M.S. (2017). *Principles of Physical Chemistry*. Jalandar: Vishal Publishing Co.
- 3) Raman, K.V. (2000). *Group Theory and its Application to Chemistry*. New Delhi: Tata McGraw-Hill.
- 4) Aruldhas, G. (2002) *Molecular Structure and Spectroscopy*. New Delhi: Prentice Hall.

Supplementary Readings

- 1) Cotton, F.A. (2008). *Chemical Applications to Group Theory*. New York: John Wiley and Sons.
- 2) Carter, R. L (2009). *Molecular symmetry and Group Theory*. New York: John Wiley and Sons.
- 3) Douglas, B. E. & Hollingsworth, C.A. (2012). Symmetry in Bonding and Spectra- an Introduction. Academic Press
- 4) Silbey, R. J., & Alberty, R. A. (2006). *Physical Chemistry*. New York: John Wiley and Sons.
- 5) Barrow, G. M. (1964). Introduction to Molecular Spectroscopy. New York: McGraw-Hill.
- 6) Banwell, C.N. & McCash, E.M. (2000). Fundamentals of Molecular Spectroscopy (4th Edition.). New Delhi: Tata McGraw-Hill.
- 7) Raman, K.V., Gopalan, R. & Raghavan, P.S. (2004). *Molecular Spectroscopy*. Singapore: Thomson and Vijay Nicol.
- 8) Levine, I. N. (1974). Molecular Spectroscopy. New York: John Wiley and Sons.
- 9) Rahman, A. (1986). Nuclear Magnetic resonance- Basic Principles. New York: Springer-verlag.

	PO1	PO2	PO3	PO4	PO5
CO1	2	3	3	2	2
CO2	3	3	3	3	2
CO3	2	3	2	2	2
CO4	2	3	2	2	3
CO5	2	2	2	3	3

SEMESTER: I		
CORE	22PCHEC14: ORGANIC CHEMISTRY PRACTICAL - I	
PRACTICAL - I		HOUK3. 70

To learn to synthesise Organic molecules with the available substrates.

Any Six preparations from the following:

- 1) p-Nnitroacetanilide from Aniline (Acetylation and Nitration)
- 2) Acetylsalicylic acid from methyl salicylate (Hydrolysis and Acetylation)
- 3) 1,3,5-tribromo benzene from aniline (Bromination, Diazotisation and Hydrolysis)
- 4) p-Bromoacetanilide from aniline (Acetylation and Bromination)
- 5) p-Bromoaniline from acetanilide (Bromination and Hydrolysis)
- 6) m-Nitrobenzoic acid from methyl benzoate. (Nitration and Hydrolysis)
- 7) p-Nitroaniline from acetanilide (Nitration and Hydrolysis)
- 8) Bezanilide from benzophenone (Rearrangement)
- 9) m-Nitrobenzoic acid from benzaldehyde (Oxidation and Nitration)

Preparations with Green chemistry procedures:

- 10) Synthesis of Salicylic acid from Methyl salicylate
- 11) Bromination of p-Bromoacetanilide from Acetanilide using CAN and KBr.
- 12) Synthesis of Anisalacetophenone from Acetophenone and p-Methoxy benzaldehyde
- 13) Synthesis of 3,5-Dimethylpyrazole from Acetylacetone and Hydrazine hydrate.(Students are expected to submit recrystallized sample of the final products at the time of practical examination for the evaluation by the examiner).

COURSE OUTCOMES

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

- 1) Acquire basic laboratory skills required to carry out organic reactions.
- 2) Independently perform two step organic preparations.
- 3) Analyse the mechanisms of reactions.
- 4) Gain the expertise to solve specific research problems.
- 5) Synthesise molecules with green chemistry procedures.

Text Books

- 1) Vogel, A. I., Tatchell, A. R., Furnis, B. S., Hannaford, A. J., & Smith, P.W.G. (2005). Vogel's Textbook of Practical Organic Chemistry (5th Ed.). Chennai: Pearson.
- 2) Mukherjee, A. (2019). Organic Chemistry with Green Chemistry. Chennai: Narosa Publishing House.

Supplementary Readings

- 1) Ahluwalia, V. K., Bhagat, P., & Aggarwal, R. (2005). Laboratory Techniques in Organic Chemistry. New Delhi: I.K. Int.
- 2) Gnanaprakasam, N. S., & Ramamurthy, G. (2000). Organic Chemistry Lab Manual. Chennai: S.V. Printers.

SCHEME OF VALUATION

Semester Examination	Marks (60)
Preparation	40
Viva - voce	10
Record	10
Total	60

	PO1	PO2	PO3	PO4	PO5
C01	2	3	3	2	3
CO2	3	3	2	2	3
CO3	3	2	2	3	2
CO4	2	2	3	3	2
CO5	3	3	3	3	2

SEMESTER: I		
CORE	22PCHEC15: PHYSICAL CHEMISTRY PRACTICAL- I	
PRACTICAL – II		HOUK5: 70

To learn the operations of instruments for calculating physical parameters.

- 1) To impart skills in evaluation of physical parameters by various methods.
- 2) To adopt different methods for validation of results.

Physical Chemistry Practical-I

- 1) Determination of cell constant-conductometric method
- 2) Conductometry-Dissociation constant of weak electrolyte (verification of Ostwald's dilution law)
- 3) Conductometry-Verification of DHO equation Equivalent conductance of strong electrolyte
- 4) Conductometric titration of HCl against NaOH.
- 5) Conductometric titration of CH₃COOH against NaOH.
- 6) Conductometric titration of NH₄OH against HCl.
- 7) Neutral salt effect Kinetics of reaction between iodide and Persulphate Effect of ionic strength on rate constant.
- 8) Polarimetry -Kinetics of inversion of Cane sugar.
- 9) Kinetics of iodination of acetone.
- 10) Kinetics of hydrolysis of ester Comparison of acid strengths.
- 11) Determination of Arrhenius parameters Hydrolysis of methyl acetate by acid.
- 12) Study of the equilibrium constant of the reaction: $KI + I_2 \leftrightarrows KI_3$.
- 13) Kinetics of decomposition of sodium thiosulphate using 0.5N HCl.

COURSE OUTCOMES

At the end of this course, the students will be able to

- 1) Interpret the experimental data of various physical parameters
- 2) Analyse the physical parameters quantitatively and qualitatively
- 3) Identify the suitable methodology to measure and characterise the physical parameters.

Text Books

- 1) Levitt, B.P. (1985). Findlay's Practical Physical Chemistry, (9th Ed.). London: Longman
- Gurtu, J. N., & Kapoor, R. (1987). Advanced Experimental Chemistry (Vol.I.). New Delhi: S. Chand & Co
- 3) Sundaram, Krishnan, Raghavan, (1996). *Practical Chemistry (Part II)* S. Viswanathan andCo. Pvt. Ltd.

Supplementary Readings

1) Shoemaker, D. P., Garland, C. W., & Nibler, J. W. (1989). *Experiments in Physical chemistry* (5th Edition.). McGraw- Hill Book company.

OUTCOME MAPPING

	PO1	PO2	PO3	PO4	PO5
CO1	2	2	2	2	2
CO2	2	3	3	3	2
CO3	3	2	2	2	3
CO4	3	2	2	3	2
CO5	2	3	3	2	2

SCHEME OF EVALUATION:

UNIVERSITY	Marks
EXAMINATION	
Procedure	10
Manipulation	15
Result	20
Record	05
Viva voce	10
Total	60

INTERNAL	Marks
ASSESSMENT	
Attendance /	20
Regularity	
Results	20
accuracy	
Total	40

- 1) To provide a thorough understanding of the basic concept of polymers
- 2) To gain knowledge about the different polymerization mechanisms
- 3) To learn the molecular weight determination and characterization of polymers.
- 4) To exploit the polymer processing techniques for various applications.
- 5) To study the importance of advanced polymers

UNIT I Introduction to polymer science

Classification - Some basic definitions - Addition and condensation polymerizations and copolymerization -. Molecular forces in polymers functionality- degree of polymerization- polymers tacticity -Polymerization techniques - Emulsion, bulk, suspension and solution polymerization. Hightemperature inorganic polymers - Preparation, properties, structure and applications of silicone polymers.

UNIT II: Kinetics and mechanism of polymerization

Polymerization - Definition - Types - Chain and step polymerization. Mechanism of ionic, radical, coordination polymerization (Ziegler-Natta catalyst), polycondensation and polyaddition polymerization. Kinetics of ionic and radical polymerization. Kinetic chain length and degree of polymerization. Copolymers -Block and graft copolymers - Kinetics of copolymerization.

UNIT III: Molecular weight and Characterization of polymers

Molecular weight of polymers - Number average and weight average molecular weight of polymers. Determination of molecular weight of polymers by GPC and Viscometry methods - Thermal analysis of polymers using DSC - Crystalline melting point (Tm) - Glass transition temperature (Tg) - Measurement of Tg - Relation between Tm and Tg - Crystallinity in polymers.

UNIT IV: Polymer processing techniques

Polymer additives - Fillers, plasticizers, stabilizers, colorants and antioxidants, lubricants - functions and examples. Compounding - Processing techniques - Calendaring, die casting, rotational casting, film casting, injection moulding, compression moulding, blow moulding, extrusion moulding, foaming, thermos-foaming, reinforcing and fiber spinning.

UNIT V: Advanced polymers

Polyelectrolytes - Conducting polymers - Biodegradable polymers - Heat resistant polymers. - Polymer blends - Polymer nanocomposites. Biomedical polymers - Artificial organs - Artificial heart, kidney, skin and cells- Contact lens -Dental polymers - Polymers for controlled drug delivery. Polymers in separation -Polymeric membranes for Reverse Osmosis, Gas separation and liquid separation.

12 hrs

12 hrs

12 hrs

12 hrs

COURSE OUTCOMES

On completion of the course, students should be able to

- 1) Understand the basic concept of polymers and the chemistry of organic and inorganic polymers
- 2) Understand the kinetics and mechanism of various polymerization techniques.
- 3) Choose an appropriate analytical method to characterize polymers.
- 4) Select an appropriate moulding technique to process a particular polymer.
- 5) Realize the importance of advanced polymers.

Text Books

- 1) Billmeyer, F. W. (2010). *Text Book of Polymer Science* (3rd Ed., Unit I to IV.). New Delhi: Gurukripa Enterprises
- Allock, H. R., Lampe F. W., & Mark J. E. (2005). Contemporary Polymer Chemistry (3rd Ed, Unit V.). Pearson Education.
- 3) Misra, G.S. (2008). Introductory Polymer chemistry. New Age International Pvt. Ltd.
- 4) Kumar. A., & Gupta, R. K. (2003). *Fundamentals of polymer engineering* (revised and expanded edition.). New Delhi: Tata McGraw Hill Publication Ltd.

Supplementary Readings

- 1) Gowariker, V. R., Viswanathan, N. V. and Sreedhar, J. (2014). *Polymer Science*. New Age International Publishers.
- 2) Fried, & Joel, R. (2000). *Polymer Science and* Technology. New Delhi: Phi Learning Pvt. Ltd.
- 3) Mathur G. N., (2000). *Recent Advances in Polymers and Composites*. New Delhi: Allied Publishers.
- 4) Sinha, R. (2002). Outlines of Polymer Technology. New Delhi: Phi Learning Pvt. Ltd.
- 5) Tager, A. (1972). Physical Chemistry of Polymers. MIR Publications.
- 6) Seymour, R. H., & Charaher, C. E., (2003). *Polymer Chemistry* (6th Ed.). Marcel Dekker Inc.
- 7) Stuart & Barbara. (2010). Polymer Analysis. New Delhi: Wiley India
- 8) Odian, G. (2007). *Principles of Polymerisation* (IV Edition.). New Delhi: Wiley Student Edition.
- 9) Arora, M. G., Singh M., & Yadav, M. S. (2003). *Polymer Chemistry* (II revised Edition.). Anmol Publications Pvt. Ltd.

	PO1	PO2	PO3	PO4	PO5
CO1	3	3	3	2	3
CO2	3	3	2	3	2
CO3	2	3	3	2	3
CO4	2	3	3	2	2
CO5	3	2	2	3	2

SEMESTER: I		CREDIT: 3
CORE ELECTIVE – I	ZZFCHEETO-Z. MATERIALS CHEMISTRT	HOURS: 60

- 1) To understand the basics of crystal structures and their defects.
- 2) To learn various crystal growth and thin-film techniques.
- 3) To study the diffusion and electronic properties of nanometrials
- 4) To gain knowledge about maganetic properties and dielectric properties of Nanomaterials.
- 5) To study Nanocomposites and their functional applications

UNIT I: Crystal structures

Crystal geometry: crystal lattices, space lattices, basis and crystal structure, unit cell, lattice parameter of a unit cell - Seven crystal systems - Bravais lattices -Crystal directions and crystal planes (Miller indices) - Coordination number, radius ratio, packing factor - Some special crystal structures - Calculation of lattice constant - Crystallographic nomenclature - Determination of crystal structure by Xray diffraction - Imperfections/defects in crystalline solids.

UNIT II: Crystal Growth and Thin film techniques

Solution growth method, melt growth method - Bridgeman method - Vapour deposition technique. Production of thin films: Thermal evaporation - Chemical vapour deposition - Spray pyrolysis - Spin coating method. Inert gas condensation, Arc discharge, RF- plasma, Plasma arc technique, Ion sputtering, Laser ablation, Laser pyrolysis, DC & RF Sputering, Molecular beam epitaxy (MBE).

UNIT III: Diffusion properties

Laws of diffusion, diffusion mechanism, ionic conductivity, relation between ionic conductivity and diffusion coefficient, experimental determination of diffusion coefficient, applications of diffusion. **Electronic Properties:** Concept of energy band diagram for materials: Conductors, semiconductors and insulators -Classification of semiconductors – Electronic conductivity - band gap determination - Hall effect and its determination. **Optical Properties:** Photoluminescence, Jablonski diagram, fluorescence and phosphorescence – Electroluminescence.

UNIT IV: Magnetic properties

Fundamentals of magnetism - Different kinds of magnetism: dia, para, ferro, ferri and anti-ferromagnetic materials - Magnetic hysteresis - Classification of magnetic materials: hard and soft magnetic materials -Super paramagnetism. **Dielectric Properties:** Effect of particles on dielectric properties, Ferro-electrics, piezo-electric, pyro-electric and muti-ferroics. **Mechanical behavior:** Stress-strain behavior, tensile strength, toughness, microhardness, wear resistance of solids materials; **Thermal properties:** Heat capacity of solids, thermal conductivity and thermal expansion of solids.

18

12hrs tal str

12 hrs

12 hrs

UNIT-V:Nanocomposites

Introduction to Nanocomposites, Types of Nanocomposites - Methods for producing Nanocomposites - Properties of Nanocomposites. **Polymer Nanocomposites:** Polymer/ Metal oxide nanocomposites - Polymer/CNTs nanocomposites - Polymer/Nanoclay-based Nanocomposites and their properties and functional applications. **Other Kinds of Nanocomposites: Fractal based** Glass- metal nanocomposites - Core-shell structured nanocomposites - Super hard nanocomposites and its designing and improvements in mechanical properties -Self-cleaning nanocomposites - Metal matrix nanocomposites and their mechanical & corrosion resistance properties and functional applications.

COURSE OUTCOME

On completion of the course the student will be able to

- 1) Understand the basics of crystal structures and their defects.
- 2) Understand the different types of crystal growth and thin film technique.
- 3) Describe the diffusion properties, electronic and optical properties of nanomaterials.
- 4) Describe various physical properties of solid/Nano- Materials.
- 5) identify various types of nano composites

Text Books

- 1) Vijaya, M. S., Rangarajan, G. *Materials Science*. New Delhi: Tata McGraw-Hill publishing company Ltd.,
- 2) Ragavan V., *Materials Science and Engineering*. New Delhi: Prentice-Hall of India(P) Ltd.
- 3) Elliott S. R. (1998). The Physics and Chemistry of Solids John. England: Wiley & Sons.
- 4) Mathur, S., & Singh, M. (2008). Nanostructured Materials and Nanotechnology (II Eds.). Willey.
- 5) Tilley, Richard J. D., (2004). Understanding Solids: The Science of Materials. John Wiley & Sons.
- 6) Koch, C. C. (2002). Nanostructured Materials. New York: Noyes Publications.
- 7) Pinnayain, T. J., & Beall, G.W. (2001). *Polymer-Clay Nanocomposites*. New York: Wiley
- 8) Chung, D. D. L. (2002). *Composite Material*. Springer. **Supplementary Readings**
- 1) Gersten, J. I., Smith, F. W., & Elliott, S. R. (1998). *The Physics and Chemistry of Materials*. New York: John Wiley & Sons.
- 2) Newnham, R. E. (2005). Properties of Materials. Oxford University Press.
- 3) Meyappan, M. (2005). Carbon Nanotubes Science and Applications. CRC Press.
- 4) Kittel, C. (2004). Introduction to solid state physics. New Delhi: Wiley India Pvt. Ltd.

5) Chattopadhyay, K. K., & Banerjee, A. N. (2014). Introduction to Nanoscience and Nanotechnology. New Delhi: PHI Learning Private Ltd.

	PO1	PO2	PO3	PO4	PO5
CO1	3	3	2	2	3
CO2	3	2	2	3	2
CO3	2	2	3	2	3
CO4	3	3	3	3	2
CO5	3	2	3	3	3

SEMESTER: I		
CORE	22PCHEE16-3: PHARMACEUTICAL CHEMISTRY	
ELECTIVE – I		HOUKS: 00

Enable the student to

- 1) Learn about the drugs and drug targets
- 2) Observe the mechanism of action of drugs and apply it for the drug design and discovery
- 3) Understand the pharmacokinetic and pharmacodynamic parameters in the drug development process
- 4) Gain knowledge about antineoplastic agents
- 5) Acquire the skill of using cardiovascular drugs for further studies.

Unit I: Drugs and drug targets: An overview

Definition of drugs, Classification of drugs, Drug targets- cell structure, at molecular level, Intermolecular boding forces- Electrostatic ionic forces, hydrogen bonds, Dipole dipole and ion dipole interactions, repulsive interactions, the role of water and hydrophobic interactions, Pharmacokinetic issues and medicine.

Unit II: Drug discovery, Design and Development

Roots of administration of drugs, biotransformation, mechanism of action. Factors prolonging action, excretion & toxicity. Development of new drugs, procedures followed in drug design, concepts of lead compound & lead modification, concepts of prodrugs & soft drugs, Structure Activity Relationship (SAR), factors affecting bioactivity, resonance, inductive effects, isosterism, bio isosterism, and spatial considerations. Theories of drug activity: Occupancy Theory, Rate Theory, induced fit theory. Quantitative Structure Activity Relationship (QSAR) - History & development. Concepts of drug receptors. Elementary treatment of drug receptor interactions.

Unit III: Pharmacokinetics

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition & in therapeutics. Uses of pharmacokinetics in drug development process. Pharmacodynamics: Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

Unit IV: Antineoplastic Agents

Introduction, classification, cancer chemotherapy, special problems, role of alkylating agents & anti metabolites in treatment of cancer. Carcinolytic antibiotics & mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards & 6-mercaptopurine. Recent developments in cancer chemotherapy. Hormone & Natural products.

12 hrs

12 hrs

12 hrs

21

Unit V: Cardiovascular Drugs

12hrs

Introduction - classification of cardiac glycosides, antiarrhythmic drugs, therapeutic uses. Antihypertensive agents, Vasopressor Drugs – Mechanism of Action. Synthesis of verapamil, methyldopa.

COURSE OUTCOMES

- 1) Identify and extend the applications of drugs and drug target.
- 2) Explain the mechanism of action drug and analyze theories of drug activity.
- 3) Interpret pharmacokinetic parameters and appraise the significance of drug metabolism in medicinal chemistry.
- 4) Classify the antineoplastic agents and integrate the synthesis of drugs to cancer therapy
- 5) Classify and predict the mechanism of action of cardiovascular drugs.

Text Books

- 1) Kar, A. (2007). Medicinal Chemistry (4th Edn.). New Age International.
- 2) Satoskar, R. S & Bharkar S. D. (2015). *Pharmacology and Pharmatherapeutics* (24th Edn.). Popular Prakasan.

Supplementary Readings

- 1) Patrick, G. L. (2009). An Introduction to Medicinal Chemistry (4th Edn.). Oxford University Press.
- 2) Sriram, D & Yogeeswari, P. (2010). *Medicinal Chemistry* (2nd Edn.) Pearson Education.

	P01	PO2	PO3	PO4	PO5
CO1	2	3	3	2	2
CO2	2	2	3	2	3
CO3	3	2	2	3	3
CO4	2	3	2	2	2
CO5	2	3	3	3	2

SEMESTER: II		CREDIT: 3
CORE: IV	22PCHEC21: ORGANIC CHEMISTRY - II	HOURS: 60

- 1) To learn about the conformations and reactivity of the substituted six membered ring systems
- 2) To understand the mechanisms of addition and elimination reactions.
- 3) To learn the name reactions with their mechanisms
- 4) To learn the synthetic utilities of various oxidation and reduction reactions.
- 5) To acquire knowledge on the various concepts of reaction kinetics and the HSAB principle.

UNIT I: Stereochemistry– II (Conformational Analysis)

Conformations of some simple 1,2 – disubstituted ethane derivatives - Gauche effect. Conformational analysis of disubstituted cyclohexane and their stereochemical features (geometrical and optical isomerism (if shown) by these derivatives). Conformation and reactivity of substituted cyclohexanol (oxidation and acylation), cyclohexanone (reduction) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis). Conformation and stereochemistry of cis and transdecalin and 9 - methyldecalin.

UNIT II: Addition Reactions

Electrophilic, nucleophilic and free radical mechanisms of addition to carboncarbon multiple bonds – isolated and conjugated multiple bonds. Hydration, hydroxylation, hydroboration. Stereochemical aspects to be studied wherever applicable. Nucleophilic addition reactions of carbonyl compounds: Perkin, Stobbe, Claisen, Dieckmann, Benzoin condensation. Mannich, Reformatsky, Grignard and Robinson Annulation.

UNIT III: Elimination Reactions

E1, E2 and E1cB mechanism - E1, E2 and E1cB spectrum - Orientation of the double bond - Hofmann and Saytzeff rules - Bredt's rule. Competition between elimination and substitution. Typical elimination reactions- dehydration, dehydro halogenation and dehalogenation. Stereochemistry of E2 eliminations in cyclohexane systems. Mechanism of pyrolytic eliminations. Chugaev and Cope eliminations.

UNIT IV: Oxidation and Reduction

Mechanism – study of the following oxidation reactions–oxidation of alcoholsuse of DMSO in combination with DCC and acetic anhydride in oxidising alcohols – oxidation of methylene to carbonyl, oxidation of aryl methanes – Etard reaction – Formation of C = C bonds by dehydrogenation, dehydrogenation by Quinones, $Hg(OAc)_2$ and $Pb(OAc)_4$. Allylic oxidation-SeO₂, Birch reduction, MPV reduction. Catalytic hydrogenation and Sommelet reaction. Selectivity in reduction of 4-tbutylcyclohexanone using selecterides. Reduction with LiAlH₄, NaBH₄, tri tertiary butoxy aluminium hydride, Sodium cyanoborohydride and trialkyl tin hydride.

12hrs

12 hrs

12hrs

UNIT V: Quantitative Treatment of Organic Reactions

Acids and Bases, HSAB, the equilibrium constant, thermodynamic and kinetic control of organic reactions. Hammond postulate, Curtin – Hammett principle. Hammett equation – Application to organic reactions. Methods of determining reaction mechanism –non-kinetic methods- Product of the presence of intermediates-isolation, detection, trapping; cross-over experiments, isotopic labelling and isotope effects, stereo chemical evidences. Kinetic methods - the relation of the rate with the mechanism of the reaction.

COURSE OUTCOMES

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

- 1) Compare the stability and reactivity of different conformers of Cyclohexane derivatives
- 2) Solve problems based on additions to Carbon Carbon and Carbon Hetero atom multiple bonds.
- 3) Propose mechanisms and predict the products with proper stereochemistry for various elimination reactions.
- 4) Have a thorough knowledge of using proper reagents for specific Oxidation and Reduction reactions.
- 5) Apply HSAB principle to Organic reactions and have sufficient knowledge on reaction kinetics and mechanism.

Text Books

- Clayden, J., Greeves, N., & Warren, S., (2012). Organic Chemistry (2nd Ed.). UK: Oxford University Press.
- 2) Smith, M. B. (2016). *March's Advanced Organic Chemistry* (7th Ed.). New York: John Wiley & Sons.
- Norman, R. O. C., & Coxon, J. M. (2003). Principles of Organic Synthesis (3rd Ed.). London (UK): Chapman & Hall.
- 4) Carey, F., & Sundberg, R. J. (2007). Advanced Organic Chemistry (5th Ed., Part A & B.). Berlin: Springer Science + Business Media.
- 5) Sykes, P. (2006). A Guide book to mechanism in organic chemistry. Pearson Edition.

Supplementary Readings

- Solomons, T. W. G., & Fryhle, C. B. (2011), Organic chemistry (10th edition.). John Wiley & Sons, Inc.
- 2) Ingold, C. K. (1994). *Structure and Mechanism in Organic Chemistry* (2nd Ed.). New Delhi: CBS Pub.
- Bansal, R. K. (1980) Organic Reaction Mechanism (2nd ed.). McGraw Hill Education India Pvt Ltd.
- 4) Mukherji, S. M., & Singh, S. P. (2016). *Reaction Mechanism in Organic Chemistry* (Revised Ed.). New Delhi: Trinity Press.

- 5) Ahluwalia, V. K., (2012). Oxidation in Organic Synthesis (1st Ed.). Florida: CRC Press.
- 6) Ahluwalia, V. K. (2012). *Reduction in Organic Synthesis* (1st Ed.). Florida: CRC Press.
- 7) Bruise, P. Y. (2002). Organic Chemistry (3rd edition). New Delhi: Pearson education.

	PO1	PO2	PO3	PO4	PO5
CO1	3	2	3	2	3
CO2	2	3	2	3	3
CO3	3	3	2	2	3
CO4	2	2	3	3	2
CO5	3	2	2	3	2

SEMESTER: II		CREDIT: 3
CORE: V	22PCHEC22: INORGANIC CHEMISTRY – II	HOURS: 60

- 1) To make the students knowledgeable in solid state chemistry.
- 2) To study about stellar energy, nuclear reactions etc and to equip the students for their future career in nuclear industry.
- 3) To learn the chemistry of lanthanides and actinides
- 4) To understand the inorganic photochemistry.
- 5) To gain knowledge about the bioinorganic complexes.

UNIT I: Solid State Structures and Structural Defects

Ionic bonding, Lattice energy, born equation and its derivation, Limiting radius ratio rules, Radius ratio for trigonal, tetrahedral, octahedral and cubic sites. Structures of some ionic crystals (sodium chloride, caesium chloride, rutile, wurtzite, fluorite). Crystal defects: Stoichiometric defects-Schottky and Frenkel defects – colour centres in alkali halide crystals – Non stoichiometric defects- metal excess and metal deficiency defects – extended defects – line and plane defects.

UNIT II:Nuclear Chemistry

Nuclear properties: nuclear spin and moments, origin of nuclear forces, nuclear models: liquid drop model and nuclear shell model. Modes of radioactive decay: Orbital electron capture, nuclear isomerism, internal conversion. Detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, Geiger-Muller, scintillation and Cherenkov counters. Nuclear reactions: Types, cross section, compound nucleus theory, high energy nuclear, direct nuclear, photonuclear and thermonuclear reactions. Stellar energy: synthesis of elements, hydrogen burning, carbon burning. Nuclear reactors: fast breeder reactors, particle accelerators, linear accelerators, cyclotron and synchrotron. Radio analytical methods: Isotope dilution analysis, radiometric titrations, radio immuno assay. Neutron activation analysis.

UNIT III: Chemistry of Lanthanides and Actinides

12 hrs

General characteristics of lanthanides-Electronic configuration-Oxidation state - Lanthanide contraction-Lanthanide contraction and its consequences-Term symbols for Lanthanide ions (Derivation not required)-Factors that mitigate against the formation of lanthanide complexes-Electronic spectra and magnetic properties of lanthanide complexes- Lanthanide complexes as shift reagents-Difference between 4f and 5f orbitals-Comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

12 hrs

UNIT IV: Photo Inorganic Chemistry

Excited states of metal complexes-Energy transfer under conditions of weak interaction and strong interaction-exciplex formation. Conditions of the excited states to be useful as redox reactants-photosubstitution, photooxidation and photoreduction- Photochemical reactions involving Ruthenium (II) bipyridyl complex. Application to photovoltaics-water photolysis- carbondioxide reduction. 12hrs

UNIT V: Bio-inorganic Chemistry

Porphyrin ring system - Metalloporphyrins - hemoglobin and myoglobin structures and work functions - synthetic oxygen carries - cytochromes - structure and work function in respiration - chlorophyll - structure - photosynthetic sequence - iron-sulphur proteins (non-heme iron protein) - Copper containing proteins – classification – blue copper proteins – structure of blue copper electron transferases - copper proteins as oxidases - Cytochrome.

COURSE OUTCOME

At the end of the course students will be able to

- 1) Explain the solid-state structures and structural defects
- 2) Explain the nuclear models, Categorize the nuclear reactions, radio analytical techniqus.
- 3) Describe chemistry of lanthanides and actinides.
- 4) Analyze and interpret the photo inorganic chemistry reactions.
- 5) Describe the chemistry of bioinorganic complexes.

Text Books

- 1) West, A. R. (1991). Basic solid-state chemistry. John Wiley.
- 2) Mallik, W. U., Tuli, G. D., & Madan, R. D. (1992). Selected topics in Inorganic Chemistry. New Delhi: S. Chand and Co.
- 3) Glasstone, S. (1969). Source Book on Atomic Energy, Van Nostrand Co.
- 4) Arnikar, H. J. (2005). Essentials of nuclear chemistry. New Age International (P) Ltd.
- 5) Lee, J. D. (1991) Concise Inorganic Chemistry. US: Springer.
- 6) Pradeep, T. (2007). Nano: The essentials. McGrew Hill Education.
- 7) Adamson. (1975). Concept of Inorganic Photochemistry. New York: Wiley.
- 8) Huheey, J. E. (1993). Inorganic Chemistry (5th Edn.). Harper International.
- 9) Purcell, M. F., & Kotz, C. (1977). Inorganic Chemistry. Saunder.
- 10) Gopalan, R. (2001). Concise Coordination Chemistry. Vikas Publishing House. Supplementary Readings
 - 1) Frielander, G., Kennedy, J. W., & Miller, J. M. (1981). Nuclear and Radiochemistry. John Wiley and Sons.
- 2) Cotton, F. A. & Wilkinson, G. W. (1988). Advanced Inorganic Chemistry A comprehensive Text. John Wiley and Sons

- 3) Shrivers, M. C., Atkins, P. W., & Langford, C. H. (1990). *Inorganic Chemistry*. Oxford University Press.
- 4) Greenwood, N. N., & Earnshaw. (1984). *Chemistry of the Elements*. New York: Pergamon Press.
- 5) Mathur, N. (2010). Nanochemistry. RBSA publishers.
- 6) Sergeev, G. B. (2007). Nanochemistry. Elsevier Science and Technology.

OUTCOME MAPPING				
	PO1	PO2		

	PO1	PO2	PO3	PO4	PO5
CO1	2	2	2	2	2
CO2	2	3	2	2	3
CO3	3	2	3	3	2
CO4	3	2	2	2	2
CO5	2	2	3	3	3

SEMESTER:	II
CORE: VI	

CREDIT: 3 HOURS: 60

COURSE OBJECTIVES

- 1) To know the foundations and the physical and mathematical basis of quantum mechanics and to apply the concepts of quantum mechanics to solve problems in microscopic systems.
- 2) To understand the quantum mechanical approach to the atomic and molecular electronic structure and to know the limitations of quantum chemistry in the evaluation of macroscopic properties
- 3) To know the mechanisms of photo chemical reaction
- 4) To know the construction of phase diagram for one, Two and three component systems
- 5) To understand the catalysis of reactions.

UNIT I: Quantum Chemistry-I

Mathematical concepts for quantum mechanics – differentiation formula for uv, u/v, (u+v), sinx, cosx, and e^x only – partial differentiation – Euler"s reciprocal relation, chain rule (statement only) – Integration methods .Inadequacy of classical mechanics-wave particle dualism – deBroglie"s equation – Uncertainty principle – postulates of quantum mechanics -significance of ψ and ψ^2 ; Schrodinger time independent wave equation-Eigen functions and Eigen values - Operators and their properties – linear and Hermitian, angular momentum operators-commutation relations.- orthogonalization and normalization. Applications of wave mechanics to simple systems – Particle in a box - one and three Dimension, Rigid Rotator-Harmonic oscillator - zero-point energy-Hydrogen atom- shapes and nodal properties of orbitals- Bohr"s correspondence principle.

UNIT II: Quantum Chemistry - II

Approximation methods – Variation method-application to one dimensional box, H_2 , H_2^+ and Helium atom -Perturbation method - application to one dimensional box and Helium atom- Born Oppenheimer Approximation-Hartree method and Hartree Fock Self-consistent Field method – many electron atoms-Pauli's principle and Slater determinant. LCAO- MO treatment of hydrogen molecular ion and H_2 -VB treatment of hydrogen molecule - hybridization of orbitals in BeF₂, BF₃, CH₄. Huckel pi-electron theory and its applications to ethylene, butadiene, benzene and allyl system.

UNIT III: Photochemistry

Differences between photochemical and thermal reactions-Quantum yield-Photophysical processes in electronically excited molecules – Jablonski diagramenergy transfer processes – Radiative and Non-Radiative transitions – Fluorescencerelation to structure- Phosphorescence- conditions for Phosphorescence emission (spin-orbit coupling)- Photosensitization – Stern - Volmer equation derivation for

12 hrs

12 hrs

quenching of luminescence and quenching of chemical reaction and its applications- Chemiluminescence.

UNIT IV: Phase Equilibrium

12 hrs

Phase diagrams for ternary mixtures-Phase rule-methods of reading and rules relating to triangular diagrams-three component system having a pair of partially miscible system-acetic acid-chloroform and water system- three component system having two pairs of partially miscible system-Water-phenol and aniline systemthree component system having three pairs of partially miscible system-succinic nitrile-water-ether system- recent applications of ternary phase diagrams in pharmaceuticals.

UNIT-V: Catalysis

12 hrs

Acid - Base catalysis - mechanism of acid - base catalyzed reactions - Bronsted catalysis law. Catalysis by enzymes - Kinetics of enzyme catalyzed reaction - Michaelis - Menten equation and its interpretation. Effect of substrate concentration, pH and temperature on enzyme catalyzed reactions - inhibition of enzyme catalyzed reactions - Competitive, Non-competitive and Uncompetitive inhibition.

COURSE OUTCOMES

At the completion of this course, the students will be able to

- 1) Identify the application of quantum chemistry in MO and VB theories and construct hybridizationschemes.
- 2) Derive the equation for one dimensional and two-dimensional boxes.
- 3) Identify the photo chemical reactions
- 4) Construct the phase diagram for the Three components system.
- 5) Illustrate the use of catalysis in reactions.

Text Books

- 1) Chandra, A. K. (2017). Introductory Quantum Chemistry. New Delhi: Tata McGraw-Hill.
- 2) Raman, K.V. (2000). *Group Theory and its Application to Chemistry*. New Delhi: Tata McGraw-Hill.
- 3) Aruldhas, G.(2002). *Molecular Structure and Spectroscopy*. New Delhi: Prentice Hall.
- 4) West, D., & Saunders, N. (2017). *Ternary phase diagrams in materials science* (3rd ed.). CRC press.
- 5) Singh, D., Deshwal, B., & Vats, S. (2007). Comprehensive engineering chemistry.
- 6) New Delhi: I K International Publishing House.
- 7) Bahl, B., Bhal, A., & Tuli, G. (2008). *Essentials of physical chemistry*. New Delhi: S. Chand & Company Ltd.

Supplementary Readings

- 1) Mcquarrie, D. A. (2016). Quantum Chemistry. University Science Books.
- 2) Levine, I. N. (2016). Quantum Chemistry. Prentice Hall.
- 3) Prasad, R.K.(2010). Quantum Chemistry. New Delhi: New Age international (P) Ltd.
- 4) Sen, B. K. (1992). Quantum Chemistry. New Delhi: Tata McGraw-Hill.
- 5) Raman, K.V., Gopalan, R., & Raghavan, P. S. (2004). *Molecular Spectroscopy*. Singapore: Thomson and Vijay Nicol.
- 6) Levine, I. N. (1974). Molecular Spectroscopy. New York: John Wiley and Sons.
- 7) Rahman, A. (1986). Nuclear Magnetic resonance- Basic Principles. New York: Springer-verlag.
- 8) Kuriakose, J. C., & Rajaram, J. C.(1999). *Thermodynamics*. Jalandar Shoban Lal Co.
- 9) Silbey, R. J., & Alberty, A. (2006). *Physical Chemistry*. New York: John Wiley and Sons.

	PO1	PO2	PO3	PO4	PO5
CO1	3	2	2	2	2
CO2	3	3	2	2	3
CO3	2	3	3	3	2
CO4	2	3	2	2	3
CO5	2	3	2	3	2

SEMESTER: II		CREDIT: 3
CORE		HOURS: 75
PRACTICAL: III	FRACTICAL - II	

- 1) To learn the methods of separating the components of an organic mixture
- 2) To analyse the organic compounds based on the organic analysis.
- 3) To identify the whether the compound is saturated or unsaturated and aliphatic or aromatic.
- 4) Confirm the particular functional group by confirmatory test.
- 5) To prepare the derivate of that particular functional group.

QUALITATIVE ORGANIC ANALYSIS

Analysis of two component mixture. Separation and systematic analysis of the separated two individual components. Preparation of their derivatives. Determination of b.p. / m.p. for components and m.p. for the derivatives.

COURSE OUTCOMES

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

- 1) Gain expertise in separating the components of an organic mixture.
- 2) Acquire the necessary practical skills to independently analyse organic compounds.
- 3) Systematically evaluate organic compounds.
- 4) Apply the knowledge in analysing new samples.
- 5) Apply the knowledge in synthesizing new molecules

Text Books

- Vogel, A. I., Tatchell, A. R., Furnis, B. S., Hannaford, A. J., and Smith, P.W.G. (2005). Vogel's Textbook of Practical Organic Chemistry (5th Ed.). Prentice Hall. New Delhi.
- 2) Gnanaprakasam, N. S., & Ramamurthy. (2000). Organic Chemistry Lab Manual. Chennai: S.V. Printers.

Supplementary Readings

- 1) Mohan, J. (2003). Organic Analytical Chemistry, Theory and Practice. New Delhi: Narosa Publishing House.
- 2) Ahluwalia, V. K., Bhagat, P., & Aggarwal, R. (2005). Laboratory Techniques in Organic Chemistry. New Delhi: I. K. International.

SCHEME OF VALUATION

Semester Examination	Marks (60)
Separation with suitable Solvent	10
Analysis of compound - 1	15
Analysis of compound - 2	15
Viva - voce	10
Record	10
Total	60

	PO1	PO2	PO3	PO4	PO5
CO1	3	2	3	2	3
CO2	2	3	2	3	2
CO3	3	3	3	2	2
CO4	2	3	2	3	3
CO5	3	2	3	3	3

SEMESTER: II		CREDIT: 3
CORE PRACTICAL: IV	22PCHEC25: INORGANIC CHEMISTRY PRACTICAL - I	HOURS: 75

To get the skill in the identification of cations including rare earth metals and to develop the skill in the preparation of metal complexes.

Semi Micro Qualitative Analysis

Mixture containing two common cations and two of the following less familiar cations.

Se, Te, W, Mo, Be, Ti, Ce, Th, Zr, U, V, Tl and Li.

Preparation of the followings:

- 1) Tris(thiourea)copper (I) chloride
- 2) Potassium trioxalatoferrate
- 3) Tetraamminecopper (II) sulphate
- 4) Microcosmic salt
- 5) Chrome alum
- 6) Trans-Diaquadioxalatochromate (III)

COURSE OUTCOMES

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

- 1) Acquire the necessary practical skills to independently analyze inorganic compounds
- 2) Gain expertise in the systematic analysis of inorganic compounds.
- 3) Apply the knowledge in industries.
- 4) Gain knowledge on the preparation of complexes

Text Books

- 1) Ramanujam, V, (1988), Inorganic Semi Micro Qualitative Analysis, National Pubs. Chennai.
- 2) Vogel, A.I. (1989), *Text Book of Quantitative Inorganic Analysis*, 5th Ed., Longman, UK.

SCHEME OF VALUATION

Semester examination	Marks (60)
Qualitative Analysis	30
Preparation	10
Viva	10
Record	10

35

	PO1	PO2	PO3	PO4	PO5
CO1	3	2	3	3	3
CO2	2	3	2	2	2
CO3	2	2	2	2	3
CO4	2	2	2	2	2
CO5	3	2	3	3	3

Enable the students to

- 1) Understand the basic principles and importance of green chemistry for industrial applications
- 2) Acquire knowledge about the microwave and ultra sound assisted synthesis
- 3) Understand the concept of phase-transfer catalysis
- 4) Gain knowledge about ionic liquids, green reagents,
- 5) Crown ethers and their applications

Unit I: Green Chemistry

Definition, need for green chemistry, basic principles, Explanation of twelve basic principles -atom efficiency process & atom economy- rearrangement, addition, substitution, elimination. Planning green Synthesis- preventing Waste, use of benign solvent, use of catalyst, minimum energy- use of polymer supported reagents. Green Synthesis in water –Wittig - Horner reaction, Heck reaction, Claisen rearrangement, Electrochemical synthesis, Weiss Cook reaction.

Unit II: Microwave Induced Green Synthesis

Introduction- microwave assisted reactions in water – Hoffmann elimination, hydrolysis, oxidation, reactions in organic solvents- esterification, Diel's Alder reaction, decarboxylation, Baylis-Hillman reaction, Knoevenagel condensation, ortho ester Claisen rearrangement, Synthesis of β - lactams, benzodiazepin-2 ones, jusminaldehyde, isopropylidene glycol and Fries rearrangement. Green reagents: Dimethylcarbamate, polymer supported reagents, Polymer supported catalysts.

Unit III: Ultrasound Assisted Green Synthesis

Introduction-Instrumentation, The physical aspects, Types of sonochemical reactions, Homogeneous sonochemical reactions, Heterogeneous liquid- liquid reactions, Heterogeneous liquid- solid reactions. Ionic liquids: Introduction, Types of ionic liquids, preparation of ionic liquids, Selection of suitable ionic liquid for a particular reaction- The Baylis- Hillman reaction in ionic liquids, Knoevenagel condensation, Claisen Schmidt condensation, Horner- Wordsworth- Emmons reaction in ionic liquids, applications in organic synthesis - Alkylation, Oxidation, hyrogenation, carbon - carbon double bond forming reactions. advantages & disadvantages of ionic liquids.

Unit IV: Phase transfer catalysts

12 hrs

Introduction, definition, mechanism of phase transfer catalysed reaction, types and advantages of phase transfer catalysts, types of phase transfer catalysed reactions, preparation of phase transfer catalysts, applications of phase transfer catalysis in organic synthesis- Nitriles, azides, alcohols from alkyl halides and addition to olefins

12 hrs

12 hrs

37

Unit V: Green Crown ethers

Introduction, nomenclature, special features, nature of donor site, general synthesis of Crown ethers -synthesis of [12] Crown- 4, [18] Crown -6 and cryptates. Synthetic applications – esterification, saponification, KMnO₄ oxidation, Elimination reaction, Generation of carbenes, and O, C-Alkylations. **synthesis in industries:** Synthesis of Adipic acid, synthesis of iburofen, synthesis of methyl methacrylate, Synthesis of sebacic acid, Synthesis of Prednisolone

COURSE OUTCOMES

- 1) Define green chemistry and explain basic principles
- 2) Discuss and appraise green reagents and microwave assisted green synthesis
- 3) Analyse the synthetic applications of ultra sound assisted green synthesis and ionic liquids.
- 4) Apprise the advantages and applications of phase transfer catalysis in organic synthesis.
- 5) Suggest crown ethers for different reactions in organic synthesis.

Text Books

- 1) Aluwalia, V. K. (2021). *Green Chemistry A Text Book* (6th reprint.). Narosa Publications.
- 2) Ahluwalia, V. K. (2012). *Environmentally Benin reactions* (2nd edn.). Ane Publications.
- 3) Ahluwalia, V. K., & Kidwai, M. (2012). *New trends in Green Chemistry* (Reprint.). Anamaya Publishers.

Supplementary Readings

- 1) Ahluwalia, V. K., & Aggarwal, R. (2012). Organic Synthesis Special Techniques (2nd edn reprint.). Narosa Publishers.
- 2) Sanghi, R. & Srivastava, M. M. (2012). *Green Chemistry: Environmentally Friendly Alternatives* (4th Edn.). Narosa Publishers.

OUTCOME MAPPING

	PO1	PO2	PO3	PO4	PO5
CO1	2	2	2	3	3
CO2	3	3	3	2	2
CO3	2	2	2	2	2
CO4	2	3	2	3	3
CO5	3	2	2	2	2

SEMESTER: II CORE	22PCHEE26-2: SUPRA MOLECULAR CHEMISTRY	CREDIT: 3 HOURS: 60
ELECTIVE-II		

- 1) To enable the students to gain knowledge about supramolecular interactions.
- 2) To enable the students to understand about the binding of Host molecules and synthesis various supramolecules.
- 3) To enable the students to visualise the bonding interactions, design, synthesis of crystal engineering of supramolecules.
- 4) To enable the students to learn the mechanism and function of supramolecules as Molecular devices.
- 5) To enable the students to acquire knowledge about biological mimics and supramolecular Catalysis.

UNIT I: Supramolecular Interactions

Definition of supramolecular chemistry. Classification of supra molecular host - guest compounds, Cooperativity and chelate effect, preorganisation and complementarity. Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation- π , anion π - π , π - π , van der Waals interactions and Closed Shell interactions.

UNITII: Binding of Hosts and Its Synthesis

Binding of cationic, anionic, ion pair and neutral Host molecules. Nomenclature of cation binding macrocycles, selectivity of cation complexation, Synthesis- The template effect and High dilution methods, Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands.

UNIT III: Crystal Engineering

Introduction, Tectons and synthons, The role of H-bonding and other weak interactions. Self-assembly in synthetic systems: design, synthesis and properties of the molecules, self-assembling coordination commounds, self-assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

UNT IV: Molecular Devices

Philosophy of molecular devices, Supramolecular photochemistry- mechanism of energy and electron transfer, Bimetallic systems and mixed Valence, Bipyridine and friends as device components, Bipyridyl type Light harvesting devices, Light conversion devices, Information and signals: Semiochemistry and sensing, molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

12 111 3

12hrs molecu

12 hrs

12 hrs

UNIT V: Biological Mimics and Supramolecular Catalysis

12 hrs

Relevance of supramolecular chemistry to mimic biological systems, Characteristics of Biological models, cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis- Abiotic supramolecular catalysis, dynamic combinatorial libraries, Self-replicating systems, Emergence of life. Examples of recent developments in supramolecular chemistry from current literature.

COURSE OUTCOMES

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

- 1) Recognize the various supramolecular interactions.
- 2) Perceive the binding of Host molecules and apply it for the synthesis of various supramolecules.
- 3) Comprehend the bonding interactions, to design the synthesis of crystal engineering of supramolecules.
- 4) Appreciate the role of supramolecular chemistry in the design of molecular device.
- 5) Identify the role biological mimics and the significant applications of supramolecular catalysis in research.

Text Books

- 1) Steed, J. W., & Atwood, J. L. (2000). *Supramolecular Chemistry*. John Wiley and Sons.
- 2) Lehn, J. M. (1995). Supramolecular Chemistry Concepts and Perspectives. Wiley-VCH.
- 3) Beer, P. D., Gale, P. A., & Smith, D. K. (1999). *Supramolecular Chemistry*. Oxford University Press.

Supplementary Readings

- 1) Ariga, K., & Kunitake, T. (2006). Supramolecular Chemistry Fundamentals and applications Advanced text Book. Heidelberg: Springer berlin.
- 2) Kubik, S. (2021). Supramolecular Chemistry- From concepts to Applications. De gruyter.
- 3) Das, A. K., & Das. M. (2017). An introduction to Supramolecular Chemistry. CBS Publications

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CREDIT: 3 HOURS: 60

COURSE OBJECTIVES

- 1) To understand the scientific background, classification and properties of nanomaterials
- 2) To gain knowledge about special nonmaterial's and to identify the bonding in nanostructure
- 3) To acquire knowledge about various methods of synthesis of nanomaterials
- 4) To learn characterization techniques used for nanosystems
- 5) To study various industrial applications of nanotechnology

UNIT I: Introduction to Nanoscience

Introduction, length scale of different structures, definition of Nanoscience and nanotechnology - Electronic structure of various nanostructures - Classification of Nanomaterials: Dimensionality and size dependent phenomena; zero-, one- and two-dimension Nano-structures; Top down and bottom-up synthesis methods - Size dependent variation in mechanical, physical and chemical, magnetic, electronic transport, reactivity etc. - Biological nanostructures, polypeptide nanowires and protein nanoparticles.

UNIT II: Special Nanomaterials

Fullerenes and Carbon nanotubes. Micro and Mesoporous Materials: Coreshell structures; **Bonding in Nanostructures:** Bonding in Graphene – Carbon Nanotubes-Inorganic nanotubes: Silica nanotubes, boron nitride nanotubes, Nanotubes of Chalcogenides, and Nanotubes of several metal oxides – Functionalization of CNTs and Graphene.

UNIT III : Synthesis of Nanomaterials

Chemical precipitation and co-precipitation, Sol-Gel synthesis; Microemulsions synthesis, Hydrothermal, Solvothermal synthesis methods, Microwave assisted synthesis; Sonochemical assisted synthesis, Quantum dot (QDs) synthesis, Bio-synthesis – Exploitation methods for the preparation of 2D Nano-materials.

UNIT IV: Nanostructured materials Characterization Techniques 12 hrs

X-ray diffraction (XRD), SEM, EDAX, TEM, FTIR, UV-Visible spectrophotometer, Laser Raman Spectroscopy, Differential Scanning Calorimeter (DSC), Differential Thermal Analyzer (DTA), Thermo gravimetric Analysis (TGA), TEM, X-ray Photoelectron Spectroscopy (XPS), Atomic force microscopy (AFM), BET alalyzer.

UNIT V: Industrial Applications of Nanotechnology

Applications of Nano-adsorbents and photocatalysts for water and wastewater treatment – Nanoparticles for degradation of solvents and organic compounds – Nanotechnology in Textiles, Cosmetics, Defence, Agriculture, and Food industry, Bio-Medical Engineering.

12 hrs

12 hrs

12 hrs

COURSE OUTCOMES

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

- 1) Discuss on the scientific background on nanomaterials
- 2) Know various methods of synthesis of nanomaterials
- 3) Know the characterization techniques used for nanosystems
- 4) Understand the properties of nanomaterials in depth
- 5) Acquire knowledge in various industrial applications of nanotechnology

Text Books

- 1) Viswanathan, B. (2014) Nano Materials. Narosa Publishing House Pvt Ltd.
- 2) Pradeep, T. (2012). *Nano: The Essentials*. Tata MC Graw-Hill Publishing Company limited.
- 3) Niemeyer, C. M., Mirkin, C. A. (2004). *Nanobiotechnology: Concepts, Applications and Perspectives*. Wiley-VCH Verlag GmbH & Co.
- Charles Poole, Jr., & Owens, F. J. (2003). Introduction to Nanotechnology. John Wiley and Sons.
- 5) Cao, G., & Wang, Y. (2011). Nanostructures and nanomaterials: synthesis, properties and applications (2nd edition.). World Scientific.
- 6) Kuzma, J., & VerHage, P. (2006). *Nanotechnology in agriculture and food production*. Woodrow Wilson International Centre.
- 7) Brown, P. J. & Stevens, K. (2007). *Nanofibers and Nanotechnology in Textiles*. Cambridge: Wood head Publishing Limited.

Supplementary Readings

- 1) Goser, K., Glosekotter, P., & Dienstuhl, J. (2005). Nanoelectronics and nanosystems: from transistors to molecular and quantum devices. Springer.
- 2) Dresselhaus, M. S., & Dresselhaus, G. (1996). Science of fullerenes and carbon nanotubes. Academic press.
- 3) Altmann, J., & Routledge. (2006). Military Nanotechnology: Potential Applications and Preventive Arms Control. Taylor and Francis Group.

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