ST.MARY'S COLLEGE (AUTONOMOUS), THOOTHUKUDI

Master of Science (Chemistry)

Course structure (w.e.f 2017)

Semester - I

Subject	Subject code	Title of the paper	Contact Hours/ week	Credits	Max. marks		
					CIA	ESE	Total
Core I	17PCHC11	Inorganic Chemistry - I	5	5	40	60	100
Core II	17PCHC12	Organic Chemistry - I	5	5	40	60	100
Core III	17PCHC13	Physical Chemistry - I	5	5	40	60	100
Core Elective I	17PCHE11	Research methodology	3	4	40	60	100
Core Practicals	17PCHCR1	Inorganic Practicals - I	4				
	17PCHCR2	Organic Practicals - I	4				
	17PCHCR3	Physical Practicals - I	4				
			30	19	160	240	400

Semester - II

Subject	Subject code	Title of the paper	Contact Hours/ week	Credits	Max. marks		
					CIA	ESE	Total
Core IV	17PCHC21	Organic Chemistry - II	6	5	40	60	100
Core V	17PCHC22	Physical Chemistry - II	6	5	40	60	100
Elective II (IDE)	17PCHE21	Industrial Products	6	5	40	60	100
Core Practicals	17PCHCR1	Inorganic Practicals - I	4	4	40	60	100
	17PCHCR2	Organic Practicals - I	4	4	40	60	100
	17PCHCR3	Physical Practicals - I	4	4	40	60	100
Self study (Compulsory)	17PCHSS1	Chemistry for National Eligibility Test - I		2	-	100	100
			30	29	240	460	700

Semester - III

Subject	Subject code	Title of the paper	Contact Hours/ week	Credits	Max. marks		
					CIA	ESE	Total
Core VI	17PCHC31	Inorganic Chemistry - II	5	5	40	60	100
Core VII	17PCHC32	Physical Chemistry - III	5	5	40	60	100
Core Elective II	17PCHE31	Phytochemistry and Photochemistry	4	4	40	60	100
Core Practicals	17PCHCR4 17PCHCR5 17PCHCR6 17PCHP31	Inorganic Practicals - II Organic Practicals - II Physical Practicals - II Project	4 4 4 4	4	40	60	100
Self study (optional)	17PCHSS2	Chemistry for National Eligibility Test - II	-	2		100	100
			30	20	160	340	500

Semester - IV

Subject	Subject code	Title of the paper	Contact Hours/ week	Credits	Max. marks		
					CIA	ESE	Total
Core VIII	17PPCC41	Nanoscience and Technology	6	4	40	60	100
Core IX	17PCHC41	Inorganic Chemistry - III	6	5	40	60	100
Core X	17PCHC42	Organic chemistry - III	6	5	40	60	100
Core Practicals	17PCHCR4 17PCHCR5 17PCHCR6	Inorganic Practicals - II Organic Practicals - II Physical Practicals - II	4 4 4	4 4 4	40 40 40	60 60 60	100 100 100
			30	26	240	360	600

SEMESTER – I			
Core I INORGANIC CHEMISTRY - I			
Code : 17PCHC11	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 5**

Unit I Structure and Bonding

Atomic orbitals - electronic configuration of atoms (L-S coupling) and the periodic properties of elements - ionic radii, ionization potential, electron affinity, electronegativity, Bond lengths, bond strength, bond angles, bond order, bond energies and lattice energy - Lewis electron dot diagrams - Hybridization, Octet rule - Resonance VSEPR theory - Walsh diagram (H_2O) - Bent's rule – Apicophilicity - Valence bond theory - MO theory of homo and heteronuclear diatomic molecules and poly atomic molecules (O_2, N_2, CO, HCl and $BeCl_2$). Geometrical isomerism - Fluxionality - Types of chemical bonds (weak and strong) - Intermolecular forces.

Unit II Coordination chemistry of transition metal ions

Stability constants of complexes and their determination, stabilization of unusual oxidation states. coordination numbers and structures, isomerism - Valence bond theory - Molecular orbital theory (sigma as well as Pi bonding) - Crystal field theory - Ligand field theory, Ligand field stabilization energy - Lattice energies and hydration energies - Irving-Williams series and the spectrochemical series - Jahn-Teller effect - nephelauxetic effect - chelate and macrocyclic effect.

Unit III Inorganic reaction mechanism

Labile and inert complexes - Thermodynamic and kinetic stability of complexes - mechanism of substitution reactions of metal complexes – D, Id, A and Ia mechanisms - Substitution reactions in octahedral and square planar complexes, acid-catalyzed reactions, base - catalyzed reactions - trans effect and its influence, water exchange, anation, isomerization reactions. Redox reactions - inner and outer sphere electron transfer mechanism - Template reactions.

Unit IV Lanthanides and Actinides:

Occurrence, properties of the elements - Common and uncommon oxidation states - Absorption and emission Spectra - magnetic properties - Separation of lanthanide elements - lanthanide and actinide contraction - similarities between actinides and lanthanides - Coordination complexes and Organometallic compounds of lanthanides and actinides - use of lanthanide compounds as shift reagents.

Unit V Spectroscopy I

IR and Raman: Selection rules - predicting number of active modes of vibrations - applications of IR and Raman in the study of inorganic structures and coordination compounds - Application of isotopic substitution, detection of intra and intermolecular hydrogen bonding.

Mossbauer: Principle, conditions for Mossbauer spectroscopy - isomer shift - quadrupole interactions - magnetic interactions - interpretation of spectra of iron and tin compounds.

References

1. James .E. Huheey, Ellen .A. Keiter and Richard .L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, Harper Collins College Publishers, 4th Edition , 1993.

2. Shriver D.F., Atkins P.W. and Langford C.H., inorganic chemistry, ELBS, Oxford university Press 1994.

3. Lee J.D., Concise Inorganic Chemistry, Blackwell Science Ltd., 5th Edition, Reprint 2003.

4. Albert Cotton F. , Geoffrey Wilkinson , Carlos .A.Manic and Manfred Bochman , Advanced Inorganic Chemistry ,Wiley Interscience Publication , 6th edition , 1999.

5. Emeleus .H.J,Sharpe. A.G., Modern Aspects of Inorganic chemistry, 4th Edition 1973

6. Wood. C.W and Holliday. A.K, Inorganic chemistry, An intermediate Text.

7. Purcell K.F. and Kotz J.C, Advanced Inorganic Chemistry, Saunders Golden Publishers

8. Skoog D.A, West D.M, Holler F.J, Grouch S.R., Fundamentals of Analytical Chemistry, Thomson Asia Pvt.Ltd.,Eighth Edition , Third Reprint , 2005 .

9. Willard H.H., .Merritt L.L and Dean J.A , Instrumental Methods of Analysis , CBS Publishers, 6th edition, 1986.

10. Handbook of instrumental techniques for analytical chemistry - Frank A. Settle, Prentice hall, 1997.

11. Drago R.S., Physical Methods in Inorganic Chemistry ,W.B.Saunders ,1977.

12. Ebsworth David E.A.V., Rankin Stephen Credock W.H., Structural Methods in Inorganic Chemistry ,ELBS , IV 1988.

SEMESTER – I			
Core II ORGANIC CHEMISTRY - I			
Code : 17PCHC12	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 5**

Unit I Reactive Intermediates and rearrangements

Carbenes - Generation, stability, structure, reactions and stereochemistry of carbenes - Wolff rearrangement and its synthetic applications.

Nitrenes - Generation, stability, reaction of nitrenes - Mechanism of rearrangements through Nitrene intermediate – Schmidt rearrangement - Hoffmann rearrangement.

Carbanion - Mechanism of rearrangements involving carbanion as intermediate Steven, Sommelet-Hauser and Favorski rearrangements.

Arynes - Generation, Structure, Stability, reactions and trapping of arynes – Cine substitution.

Unit II Aliphatic Nucleophilic and Electrophilic Reactions

Aliphatic Nucleophilic Substitution - SN1 and SN2 mechanisms - effect of substrate structure, leaving group, attacking nucleophile and solvent polarity - Neighbouring group participation - substitution at vinylic and allylic carbons and reactivity - Ambient nucleophiles and substrates - Hydrolysis of esters.

Electrophilic substitution – SE1 and SE2 mechanism-effect of substrate structure, leaving group and solvent polarity.

Unit III Aromaticity and Ring system

Aromatic character – Huckel's rule – Aromatic , Antiaromatic, and Non aromatic – Molecular orbital description of aromaticity, antiaromaticity and homoarmaticity - Aromatic and antiaromatic ions – Alternate and Non-alternate hydrocarbons - Antiaromatic compounds – Paratopic compounds - Aromaticity of azulene - Tropones – Annulene - Higher annulenes - Fullerenes – Sydnones –Nomenclature of Bicyclic and tricyclic systems – Structure, stereochemistry and synthesis of Adamantane, Diamantane and Cubane.

Unit IV Study of Organic reaction mechanism

Reaction mechanism – Transition state and intermediate - Kinetic and Thermodynamic requirements of reactions – Hammond Postulate and microscopic reversibility - Kinetic and Thermodynamic control of product formation - Kinetic and Non- kinetic methods of determination – Primary and secondary isotope effect - Testing and Trapping of intermediates, Isotopic labeling, Cross-over experiments and stereo chemical evidence - LFER - Hammett equation – Physical significance of σ and ρ – Applications and Limitations – Taft equation.

Unit V Stereochemistry

Molecular symmetry and Chirality - Types of molecules exhibiting optical activity - Configurational nomenclatures of acyclic and cyclic molecules - cis-trans and E-Z and D-L; R-S; erythro and threo; syn and anti; endo and exo.

Stereochemistry of molecules with axial chirality - atropisomerism – biphenyls, allenes, spiranes and analogues - Helicity and Chirality - Topocity and Prostereoisomerism - Topocity of ligands and faces - Enantiotopic ligands and faces - Diastereotopic ligands and faces - Racemization methods - Mechanisms of racemization through carbocations, carbanions and freeradicals - Resolution - Methods of resolution.

Reference:

1. Ahluwalia V.K and Parshar R.K, Organic Reaction Mechanism Fourth Edition , Narosa Publishing House, 2013.
2. Kalsi P S, Stereochemistry: Conformation and Mechanism, 4th Edition, New-Age International Publishers, New Delhi (1997).
3. Morrision R.T. and Boyd R.N., Organic Chemistry, Seventh Edition, Allyn & Bacon Ltd., New York (2011)
4. March J, Advanced Organic Chemistry, Fourth Edition, John-Wiley andSons, New York (1992).
5. Eliel E L, Stereochemistry of Carbon Compounds, Tata-McGraw Hill Publishing Company, New Delhi (1975).
6. Nasipuri D, Stereochemistry of Carbon Compounds, Third Edition, New-Age International Publishers, New Delhi (2011).
7. Sykes P, Guide Book to Mechanism in Organic Chemistry, Third Edition,ELBS with Longmann (1988).
8. Finar I L, Organic Chemistry Volume I and II, Sixth Edition, Pearson Education Ltd., (2011).
9. Michael B.Smith, Organic Synthesis, McGraw Hill Publishing Company (1994).
10. Francia.A.Carey, Organic Chemistry, Third Edition, Tata-McGraw Hill Publishing Company, New Delhi (1999).
11. Clayden, Greeves,Warren and Wothers, Organic Chemistry, Oxford University Press, New York (2006).

SEMESTER – I			
Core III PHYSICAL CHEMISTRY - I			
Code : 17PCHC13	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 5**

Unit I Quantum Mechanics I

Limitation of classical mechanics and success – Plank's quantum theory – Compton effect – wave particle duality – Uncertainty principle - Operators and their algebra - Eigen value and Eigen functions - Quantum mechanical postulates - Schrodinger equations (Time dependent and Time independent), Particle in a box (1D and 3D) - Quantum mechanical tunneling and transmission coefficient - Rigid rotor and simple harmonic oscillator.

Unit II Quantum Mechanics II

Approximation methods - Variation theorem - Application of variation method to hydrogen and helium atoms - Perturbation theory (First order) - Application to helium atom - Pauli exclusion principle - Slater determinant and HF-SCF methods to He atom - Born-Oppenheimer approximations – LCAO-MO and VB treatments of H_2 molecul - Huckel theory - application to ethylene, butadiene and benzene -Calculation of electron density and bond order.

Unit III Electrochemistry I

Debye-Huckel theory of inter-ionic attraction – Debye-Huckel-Onsager equation and its validity- Debye –Falkenhagen and Wein effects - Debye-Huckel limiting law - Debye-Huckel Bronsted equation - Quantitative and qualitative verification of Debye-Huckel limiting law - Electrode-electrolyte interface - Electrical double layer - Electrocapillary phenomenon - Lipmann equation.

Unit IV Electrochemistry II

Polarization and overpotential - Butler-Volmer equation for one step and multistep electron transfer reactions - Tafel equation - Significance of I_c and transfer coefficient – polarizable and non polarizable interface – Mechanism of metals-hydrogen and oxygen evolution reactions - Corrosion and Polarization of metals - Pourbaix diagrams - Evan's diagram - Fuel cells - Electrode deposition – Principle and applications.

Unit V Macromolecules

Polymerization in homogeneous and heterogeneous phases – Kinetics and mechanism of addition polymerization (Free radical and cationic) and condensation – kinetics of copolymerization – Properties of polymers - glass transition temperature and crystallinity of

polymers. Molecular weights – Distribution and methods of determination - light scattering, ultracentrifuge, viscosity, osmometry and gel permeation chromatography. Conducting polymers - Factors affecting the conductivity of conducting polymers - doping of conducting polymers - solitons , polarons and bipolarons.

References

1. Moore.W.J - Physical chemistry, Prentice-Hall of India Pvt. Ltd.(1962).
2. Castellan.W - Physical chemistry,
3. Atkins.P.W - Physical chemistry , ELBS edition of third edition (1987)
4. Prasad R K, Quantum Chemistry, Ist Edition, New Delhi, Wiley Eastern Ltd, (1992).
5. Donald A McQuarrie, Quantum Chemistry, Indian Edition, Viva Books PrivateLtd.
6. Chandra A K, Introductory Quantum Chemistry, Fourth Edition, Tata McGraw, Hill (1994).
7. Levine I N, Quantum Chemistry, Fourth Edition, Prentice Hall of India,Pvt. Ltd (1994).
8. Atkins P W, Molecular Quantum Mechanics, Clarendon (1973).
9. Anatharaman R, Fundamentals of Quantum Chemistry, McMillan, NewDelhi (2001)
10. Antorpov L, Theoritical Electrochemistry, Mirpublishers, Moscow.
11. Bockris J O'M and Reddy A K N, Modern Electrochemistry Vol 1 & 2,Second Edition, Plenum Press, New York (1998).

    Glasstone S, An Introduction to Electrochemistry, New Delhi, East West Press Pvt. Ltd, (1956).

SEMESTER – I			
Elective I RESEARCH METHODOLOGY			
Code : 17PCHE11	**Hrs / Week : 3**	**Hrs / Sem : 45**	**Credits : 4**

Unit I Research methodology I

Introduction of research - selection of a research topic - reviewing the literature - including patents - primary source – secondary source – including reviews, treatise and monographs – Abstraction of research papers – possible ways of getting oneself familiar with current literature - preparing the proposal and design of study - Experimentation and interpretation of results - Survey of literature - Applications of Microcal origin and Chemdraw.

Unit II Research methodology II

Identification of research problem – assessing the status of the problem guidance from the supervisor – actual investigation and analysis of experimental results – conclusions – presenting scientific seminar – reporting the results in the form of communication, paper etc-dissertation and thesis writing.

Idea of writing research articles – project proposals to the funding agency - Search engine for locating information and chemical data bases - E-mail operation and online submission of manuscript for publication.

Unit III Spectroscopic techniques

Types of atomic spectroscopy – Absorption, emission and fluorescence methods – Applications of atomic spectroscopy.

Principle, instrumentation and data interpretation of Transmission electron microscopy (TEM), Scanning electron microscope (SEM), Energy dispersive spectroscopy (EDAX), and X-ray diffraction (XRD) analysis.

Unit IV Chromatographic techniques

Principle, instrumentation and specific applications of Column chromatography, Thin layer chromatography, Gas Chromatography (GC), High Performance Liquid Chromatography (HPLC), Size-Exclusion Chromatography (SEC), Ion Chromatography (IC) - Capillary Electrophoresis - Hyphenated techniques - Introduction to interfaces, principle, instrumentation and applications of GC-MS, LC-MS and GC-FT-IR.

Unit V Data analysis

Errors in chemical analysis – classification of errors – determination of accuracy of methods – improving accuracy of analysis – significant figures – mean, median and standard

deviation – comparison of results - “t” test, “f” test and “chi” square test – rejection of results – presentation of data - Correlation and linear regression.

References

1. Mahadevan. C, Research Methodology, Sakuntala Publications, Nagercoil, 1st edition, 2000.
2. Anderson. J, Durston. B. H, Poole. M, Thesis and Assignment Writing, Wiley Eastern, New Delhi, 1986.
3. Bottle. R.T, The Use of Chemical Literature, Butterworths, 1969.
4. Durston. A.J, Thesis and Assignment Writing.
5. Butlet. R.O, Preparing Thesis and Other Manuscripts.
6. Skoog. D.A, Holler. F.J and Nieman. T.A, Principles of Instrumental Analysis, Thomson, 5th edition, 6th reprint 2005.
7. Skoog. D.A, West. D.M F, Holler. J, Crouch. S.R, Fundamentals of Analytical Chemistry, Thomson Asia Pvt. Ltd., Eighth Edition, Third Reprint, 2005.
8. Sharma. B.K, Instrumental Methods of Chemical Analysis, Goel Publishing House, 23rd edition 2004.
9. Kopkar. S. M, Basic concepts of analytical chemistry
10. Das and Behera, Experimental Chemistry, Tata McGraw Hill, New Delhi.
11. Willard. H, Merrit Jr. L and Dean. A, Instrumental methods of analysis.
12. Banwell. C.N, Fundamentals of molecular spectroscopy.
14. http://www.dst.gov.in/whats_new/whats_n07/tsd-format.pdf
15. http://www.ugc.ac.in/financialssupport/xiplan/mrpxiplan.pdf

SEMESTER – II			
Core IV ORGANIC CHEMISTRY - II			
Code : 17PCHC21	**Hrs / Week : 6**	**Hrs / Sem : 90**	**Credits : 5**

Unit I Aromatic Electrophilic and Nucleophilic substitution reaction

Aromatic Electrophilic substitution - Arenium ion mechanism – Selected reactions and Reactivity - Nitration - Nitrosation - Sulphonation – Halogenation - Friedel Craft's alkylations and arylations - Vilsmeir Haack reaction - Jacobsen reaction - Bischler Napieralski reaction - Pechman reaction – Houben Hoesch reaction.

Aromatic Nucleophilic Substitution - SNAr mechanism - SN1 (Aromatic) mechanism with evidences - Benzyne mechanism - effect of substrate structure, leaving group, attacking nucleophile and solvent - Selected reactions - Von Richter and Smiles rearrangements.

Unit II Addition and Elimination reaction

Addition to C-C bonds - electrophilic, nucleophilic and free-radical additions - Additions to conjugated systems – Birch reduction – hydroboration - Michael condensation – Diels-Alder reactions - Carbene addition to double bonds - hydration of olefins.

Mannich reaction - Meerwein-Pondorf reduction – Aldol - Claisen – Stobbe - Darsen – Wittig – Thorpe and benzoin condensations - Cannizaro reaction - Elimination reactions - E1, E2 and E1CB mechanisms – orientations - Hofmann and Saytzeff rules - Elimination versus substitution - Chugaev reaction – Cope elimination - dehydration of alcohols – dehydrohalogenation - mechanism and orientation in pyrolytic elimination.

Unit III Reagents in organic reactions

Synthetic applications of the following - Gilman, DDQ, DCC, PCC,1,3-dithiane, Fetizon's reagent, Lemieux-Johnson reagents, Prevost and Woodward reactions, Jones reagent, Bio-oxidants (Pseudomonas putida), Wilkinson's catalyst, Ziegler-Natta catalyst.

UNIT – IV Retrosynthetic analysis

Synthon - synthetic equivalent – Functional group interconversions - use of protecting groups for alcohols, amines, acids, carbonyl compounds - Use of activating and blocking groups - Robinson annulations reaction - Carbon skeletal complexity - Role of key intermediates in organic synthesis - Reterosynthetic analysis of the following compounds - Twistane, cis–Jasmone, Baclofan, Brufen, Trihexylphenydyl, Bisabolene, a-onocerin, isonootkatone, cascarillic acid, camphor and 2,4- dihydroxy pentanoic acid.

Unit V Molecular rearrangement

Migration of Carbon – Wagner-Meerwein rearrangement - Pinacol-Pinacolone rearrangement - Benzil-Benzilic acid rearrangement - Dienone- Phenol rearrangement.

Migration of heteroatoms - Migration to electron deficient nitrogen – Beckmann rearrangement and Lossen rearrangement. Migration to electron deficient oxygen – Baeyer-Villiger oxidation - Hydroperoxide rearrangement - Dakin reaction. Migration to electron rich carbon – Neber rearangement Tiffenev—Demjanov rearrangement.

References

1. Sykes P, Guide Book to Mechanism in Organic Chemistry, Sixth Edition,ELBS with Longmann (1997).
2. Finar I L, *Organic Chemistry* Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).
3. Morrision R.T. and Boyd R.N., Organic Chemistry, Sixth Edition, Allyn & Bacon Ltd., New York (1976)
4. March J, Advanced Organic Chemistry, Fourth Edition, John-Wiley andSons, New York (1992).
5. Ahluwalia V.K and Parshar R.K, Organic Reaction Mechanism Second Edition , Narosa Publishing House , 2005
6. Norman R.O.C, J.M. Coxon, Principles of Organic synthesis, Third edition, Chapman and Hall , 1994.
7. Michael B.Smith, Organic Synthesis, McGraw Hill Publishing Company (1994).
8. Kalsi P S,Organic Reaction & Mechanism, 4th Edition,New-Age International Publishers, New Delhi (2010).
9. Clayden, Greeves,Warren and Wothers, Organic Chemistry, Oxford University Press, New York (2006).

SEMESTER – II			
Core V PHYSICAL CHEMISTRY - II			
Code : 17PCHC22	**Hrs / Week : 6**	**Hrs / Sem : 90**	**Credits : 5**

Unit I Symmetry properties of molecules and Group Theory

Symmetry elements and symmetry operations - Principles of group theory (point groups) – postulates and types of group - symmetry and dipole moment - symmetry and optical activity - symmetry operations as a group multiplication table - Point group - Schoenflies symbols – Matrix representations of operations - Great orthogonality theorem - Reducible and irreducible representations - Construction of character tables for point groups (C_{2v}, C_{3v} and D_{2h}) - Explanations for the complete character table for a point group.

Unit II Applications of Group Theory

Applications of Group theory - Standard reduction formula relating reducible and irreducible representations - Hybridization schemes for atoms in molecules of different geometry (AB_4 tetrahedral, AB_3 triangular planar, AB linear molecules) - Symmetries of vibrational modes in non-linear molecules (H_2O, NH_3 and BF_3) - Symmetries of vibrational modes in linear molecules (HCN, CO_2, C_2H_2) -Integration method - Selection rules in spectroscopy - Mutual exclusion rule.

Unit III Surface Chemistry

Surface phenomenon – Physical and chemical adsorption - Adsorption and free energy relations at interface - Langmuir adsorption isotherm – Gibbs adsorption isotherm - BET isotherm - Measurement of surface area - Heterogeneous catalysis - Mechanism - Langmuir-Hinshelwood Mechanism - Langmuir- Rideal bimolecular mechanism - Role of surface in catalysis.

Unit IV Introduction of spectroscopy and Rotational spectra

Characterization of electromagnetic radiation - Regions of spectrum - transition probability - width and intensity of spectral transitions.

Classification of molecules according to their moment of inertia - Rotational spectra of rigid and non rigid diatomic molecules - The intensities of spectral lines - The effect of isotopic substitution - Polyatomic and symmetric top molecules - Stark effect.

Unit V Infrared spectroscopy and Raman spectroscopy:

Infrared spectroscopy – Polyatomic molecules - Fundamental vibrations and their symmetry - overtone and combination frequencies - concept of group frequencies - Fermi resonance and FT-IR.

Raman Spectroscopy – Rayleigh scattering - Raman Scattering - classical and quantum theories of Raman effect - Rotational Raman spectra for linear and symmetric top molecules - Vibrational Raman spectra - rotational fine structure - Polarization of light and the Raman effect - Technique and instrumentation - Laser Raman spectrometer - Structure determination from Raman and Infra-red spectroscopy.

References

1. Cotton. F.A - Chemical applications of group theory. Wiley Third edition (2003).
2. Raman K V, Group Theory and its Applications to Chemistry,Tata McGraw HillCo. (1994).
3. Arthur W.Adamson , Physical Chemistry of Surfaces , John Wiley and Sons , INC
4. B. P. Straughan and S. Walker - Spectroscopy (vol. I).
5. Banwell C N, Molecular spectroscopy, New Delhi, TATA McGraw HillCo. (1997).
6. Drago R S, Physical Methods in Inorganic Chemistr, New Delhi, East West Press Ltd, (1971).
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9. Barrow G M, Introduction to Molecular Spectroscopy, Tata McGraw Hill Edition (1993).
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11. Silvertein R. M and Basseler G. C, Spectroscopic identification of organic compounds.

SEMESTER – II			
Inter Disciplinary Elective INDUSTRIAL PRODUCTS			
Code : 17PCHE21	**Hrs / Week : 6**	**Hrs / Sem : 90**	**Credits : 5**

Unit I Cosmetics and Personal Care

Cosmetic formulations – Skin care - Hair care - Deodarants and Antiperspirants - Colour cosmetics - Sun protection aerosols - Nail cosmetics - Mouth cosmetics - Perfumes and fragrances.

Basic ingredients - Additives and flavours used in soaps, tooth pastes, lipsticks, perfumes, colognes, deodorants and antiperspirants - Harmful beautifying practices and their chemistry (Keratin depletion in hair – colouring - cleaning and curling of hair) - Basic tests for identifying good and bad cosmetics – pH Test.

Unit II Fuels and Combustion

Introduction - Calorific value - Characteristics of a good fuel - Classification of fuels - Solid (primary and secondary), Liquid (primary and secondary) and Gaseous (Natural gas, Bottled gas, Blast furnace gas) – Non-petroleum fuels – Nuclear fuel – Petrochemicals – Combustion - Flue gas analysis.

Unit III Alloys and Corrosion

Alloys – Introduction - General characteristics of Alloys – manufacture – purpose of alloying - the Iron-Carbon Alloys - Carbon steels - Types of alloys - Heat treatment of alloys (Hardening of steel and Annealing) – Steel - Alloy steel – Stainless steel – Cast iron – Brass – Bronze – Nichrome.

Corrosion – Definition - Rusting of iron - Chemical corrosion - electrochemical corrosion - Factors influencing corrosion - Atmosperic and soil corrosion - Corrosion control - Hot dipping (galvanizing and tanning), Electroplating and Anodizing.

Unit IV Pigments, Dyes and Paints

Pigments – Classification - Manufacture and uses of White lead, Lithopone, Ultramarine blue, Chrome green.

Dyes – Classification, preparation and dyeing processes.

Paints – Composition, manufacture and testing of paints - Special paints – temperature indicating paints, fire retardant paints, water repellant paints.

Unit V Macromolecules

Polymerisation – Definition, classification of polymers – Types of polymerization – Difference between addition and condensation polymerization – Kinetics of free radical polymerization – Glass transition temperature – Plastics – characteristics of plastics – Classification – Difference between thermoplastic resin and thermosetting resin – Preparation, properties and uses of PVC, Teflon and Phenol-formaldehyde resin – Plymer processing – Fabrication of plastics – Processing techniques – Compression moulding, Injection, Extrusion, Transfer and Blow techniques.

References

1. Kirpal Singh, Chemistry in Daily Life, Prentice Hall of India Pvt. Ltd., New Delhi, 2nd Edn., 2008.
2. Seema Yadav, "Food Chemistry", Anmol Publishing (P) Ltd., New Delhi, 2000.
3. Alex V. Ramani. "Food Chemistry" MJP publishers, Chennai, 2009.
4. Charkarabarthy.B.N, Industrial Chemistry, Oxford and IBH Prb.Co.
5. Sharma B.K, Industrial Chemistry, Goel Publishing House.
6. Jain & Jain, Engineering Chemistry, S.Chand Publications, New Delhi.
7. Siva kumar.R, Siva Kumar. N, Engineering Chemistry, The Mc Graw- Hill companies, New Delhi.
8. Gopalan.R,Venkappayya .D, Sulochana Nagarajan, Engineering Chemistry II, Vikas Publications,New Delhi, 2011.
9. V. Srinivasa, S.D.Uma Mageswari, M.Meena, Engineering Chemistry, Scitech Publications, 2002.

SEMESTER – II	
Self Study CHEMISTRY FOR NATIONAL ELIGIBILITY TEST - I	
Code : 17PCHSS1	**Credits : 1**

Inorganic Chemistry

1. Chemical periodicity
2. Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory).
3. Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties
4. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.
5. Organometallic compounds: synthesis, bonding and structure, and reactivity.
6. Analytical chemistry- separation, spectroscopic, electro- and thermoanalytical methods.
7. Bioinorganic chemistry: metalloenzymes, metal complexes in medicine.
8. Characterisation of inorganic compounds by IR, Raman, Mössbauer, UV-vis, MS, electron spectroscopy and microscopic techniques.

Organic Chemistry

1. IUPAC nomenclature of organic molecules including regio- and stereoisomers.
2. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
3. Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.
4. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.
5. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
6. Common named reactions and rearrangements – applications in organic synthesis.
7. Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.

Physical chemistry

1. Basic principles of quantum mechanics: Postulates; operator algebra; exactly-solvable systems: particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta; tunneling.
2. Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy; applications.
3. Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle.
4. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems.
5. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.
6. Chemical thermodynamics: Laws, state and path functions and their applications; thermodynamic description of various types of processes; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.
7. Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.
8. Polymer chemistry: Molar masses; kinetics of polymerization.
9. Data analysis: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

SEMESTER – I & II			
INORGANIC PRACTICALS - I			
Code : 17PCHCR1	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Qualitative analysis of inorganic mixture containing two familiar and two less familiar cations Pb, Cu, Bi, Cd, Sb, Zn, Co, Ni, Mn, Ca, Ba, Sr, W, Tl, Te, Se, Mo, Ce, Th, Zr, V, U, Ti and Li.
2. Complexometric titrations – Estimation of Cu, Zn and Mg by EDTA titration in presence of either Pb or Ba.

COURSE WORK

1. Photocolorimetric estimation of Fe, Ni, Cr, Mn, Cu and NH_4^+.

Reference

1. Revised by Svehla. G, Vogel's Qualitative Inorganic Analysis, Pearson Education, 7th edition.

SEMESTER – I & II			
ORGANIC PRACTICALS - I			
Code : 17PCHCR2	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Micro Qualitative Analysis of an organic binary mixture

i. Pilot separation
ii. Bulk separation
iii. Determination of melting and boiling points
iv. Analysis of organic compounds
v. Derivatization

2. Preparation of Organic compounds

1. Preparation of Benzoic acid from benzyl Chloride.
2. Preparation of Resacetophenone from resorcinol.
3. Preparation of dibenzalacetone from benzaldehyde.
4. Preparation of 2,4,6-tribromoaniline from aniline.
5. Preparation of Tetrahyrocarbazole from cyclohexanone.
6. Preparation of Iodobenzene from aniline.

3. Course work

Chromatographic techniques

i) TLC
ii) Paper chromatography

References

1. B.S. Furniss, A.J. Hannaford, P.W.G. Smith, and A.R. Tatchell, Vogel's Textbook of Practical Organic Chemistry, V Edition, Pearson Education Ltd., (2008).
2. Ganapragasm and Ramamurthy, Organic Chemistry Lab Manual, Second Edition, S. Vishwanathan Printers and Publishers (P) Ltd., Chennai (2007).
3. Ragupathi Mukhopadhyay, Pratul Chatterjee, Advanced Practical Chemistry, Books and Allied (p) Ltd., Third edition, (2007).

SEMESTER – I & II			
PHYSICAL PRACTICALS - I			
Code : 17PCHCR3	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

A. Distribution

1. Distribution of Benzoic acid between Benzene / Toluene and Water.
2. Determination of K_a by using Ostwald distribution method.

B. Conductivity

3. Determination of solubility product of a sparingly soluble salt
4. Titrations

   i) HCl + CH_3COOH vs NaOH

   ii) HCl + NH_4Cl vs NaOH

   iii) CH_3COOH + CH_3COONa vs NaOH

   iv) CH_3COOH + CH_3COONa vs HCl

C. Kinetics

5. Study of primary salt effect on $K_2S_2O_8$
6. Kinetics of $K_2S_2O_8$ and I_2

D. Thermometry

7. Determination of solution enthalpy

   i) Oxalic acid – Water

   ii) Ammonium oxalate – Water

   iii) Naphthalene – Toluene

References

1. Viswanathan.B and Raghavan.P.S , Practical Physical Chemistry , Viva Books Pvt.LTD.,(2005)
2. Michell.J.Sienko, Robert.A. Plane , Stanley.T. Martu , Experimental Chemistry, International student edition (`1984)
3. David . P. Shoemaker, Carl. W. Garland and Joseph.W.Nibler , Experiments in Physical Chemistry, McGraw Hill International edition
4. Levitt.B.P , Findlay's Practical Physical Chemistry , Edition IX
5. Yadav. J.P , Physical Chemistry Practicals
6. Peter Mathews.G , Experimental Physical Chemistry , Clarendan Press Oxford(1985)

SEMESTER – III			
Core VI INORGANIC CHEMISTRY - II			
Code : 17PCHC31	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 5**

Unit I Solid state I

Electronic structure of solids - band theory, free electron theory, Insulators and semiconductors and its types. Electrical properties (Thomson effect, Peltier effect, Seeback effect, Hall effect) - Dielectric, Ferroelectric, Piezoelectric and Pyrroelectric materials and their and applications. Optical and magnetic properties of semiconductors, p - n junction and n-p-n junction and their applications. Solid electrolytes, superconductors, High-temperature superconductors, BCS theory, cooper electrons Meissner effect and levitation.

Unit II Solid state II

Types of close packing - hcp and ccp, packing efficiency, radius ratios - Powder x-ray diffraction - electron and neutron diffraction – Solid state reactions - Methods of Single crystal growth- Bridgeman, Czochralski, Verneuil - Chemical vapour transport - Hydrothermal method - Dislocations in solids - Point defects - Schottky and Frenkel defects - Line defects - Surface Defects – Dislocations - Grain Boundary and Stacking Fault - Crystal structures of common ionic compounds NaCl, Na_2O, zinc blende, wurtzite, nickel arsenide, CsCl, rutile, CdI_2, $CdCl_2$, and Cs_2O, perovskite, K_2NiF_4, spinels.

Unit III Nuclear Chemistry

Radioactive decay and equilibrium - Nuclear Reactions - Types, Q value, Cross Section of reactions, Chemical effects of nuclear transformation - Nuclear Fission - theory of nuclear fission, Fission Products, Fission Yield - Nuclear Fusion and stellar energy - Nuclear Reactors - Nuclear waste management - Nuclear reactors in India – Radioactive techniques: i) Countering Techniques such as G.M Ionization and Proportional counters. ii) Tracer techniques (Neutron activation analysis).

Unit IV Spectroscopy II

Electronic spectroscopy - Microstates, Term symbols, selection rules - Orgel and Tanabe sugano diagrams - charge transfer spectra - electronic spectra of complexes (transition and inner transition complexes) - Calculation of Dq, B, Nephelauxetic ratio.

Photo electron spectroscopy – UVPES - Principle, spin-orbit coupling – XPES - Principle, spin- spin splitting , chemical shift in XPES - Koopman's theorem - Applications of XPES and UVPES to inorganic spectra - Auger electron spectroscopy.

Unit V Spectroscopy III

NMR - Principle, ^{31}P, ^{19}F and ^{15}N NMR - Applications of spin-spin coupling to structure determination - Nuclei with quadrupole moment - Double resonance - NMR of fluxional molecules - Applications in biological systems.

NQR – Principle - Energies of the quadrupole transitions - Structural information from NQR spectra.

EPR – Principle - Interaction between nuclear spin and electron spin (hyperfine coupling) - Hyperfine splitting in isotropic systems - Zero field splitting - Kramer's degeneracy - Anisotropy in the g value - Interpretation of g values - Anisotropy in hyperfine coupling - Applications to transition metal complexes - Jahn - Teller distortion.

References

1. West A.R., Solid State Chemistry and its Applications, John Wiley & Sons (Asia), 1998.
2. Azaroff L.V., introduction to solids, Tata McGraw Hill publishing Ltd.
3. Kittel C., Introduction to solid state physics, Wiley Eastern Ltd, 5th Edn.
4. Samuel Glasstone, Source Book of Atomic Energy, East West Pvt.Ltd., 1969.
5. Arnikar H.J, Essentials of Nuclear Chemistry, Wiley Eastern Ltd., 4th Edition, 2000.
6. Lee J.D., Concise Inorganic Chemistry, Blackwell Science Ltd., 5th Edition, Reprint, 2003.
7. Drago R.S., Physical Methods in Inorganic Chemistry ,W.B.Saunders, 1977.
8. Ebsworth David E.A.V., Rankin Stephen Credock W.H., Structural Methods in Inorganic Chemistry ,ELBS , IV 1988

SEMESTER – III			
Core VII PHYSICAL CHEMISTRY - III			
Code : 17PCHC32	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 5**

Unit I Chemical Kinetics

Theories of reaction rates - Arrhenius theory - Hard-sphere collision theory of gas phase reactions - Potential energy surfaces - Activated complex theory for ideal gas reactions (formation in terms of partition functions) - Relation between activated complex theory and hardsphere collision theory - Thermodynamic formulation - Activated complex theory (Enthalpies and entropies of activation) - Unimolecular reactions - Lindemann, Hinshelwood, RRK, RRKM and Slater theories - Kinetic isotopic effect.

Unit II Statistical Thermodynamics

Quantum statistics – Maxwell-Boltzmann statistics - Thermodynamic probability - Thermodynamic probabilities of systems in equilibrium - Boltzrnann expression for entropy – Stirling's approximation - States of maximum thermodynamics probability - Legrangian multipliers - Thermodynamic probabilities of systems involving energy levels – Maxwell-Boltzmann distribution law - Evaluation of alpha and beta in MB distribution law.

Unit III Applications of Statistical Thermodynamics

Partition function - Definition, justification of nomenclature, microcanonical and canonical ensembles - Molecular partition function and canonical function - The relation between the total partition function of a molecule and the separate partition functions - Translational partition function, rotational partition function - Effect of molecular symmetry on rotational partition function - Ortho and para hydrogen - Vibrational partition function - Electronic partition function - Evaluation of thermodynamic properties E, H, S, A, G, Cv and Cp from monoatomic and diatomic ideal gas molecule partition functions.

Unit IV Electronic Spectroscopy

Electronic spectroscopy of diatomic molecules - Born-Oppenheimer approximation - Sequences and progressions - Vibrational course structure and rotational fine structure of electronic band – The Frank-Condon principle - Dissociation energy and dissociation products - Birje-Sponer extrapolation - The fortrat diagram – Predissociation.

Photoelectron spectroscopy – Principle - Basic idea - X-ray and UVPES - ESCA - Applications of Auger electron spectroscopy.

Unit V NMR and ESR

Nuclear Magnetic Resonance Spectroscopy - Theory of PMR spectra - Chemical shift - Factors affecting chemical shift - Relaxation times and spin-spin interactions - NMR of simple AX and AMX type molecules - Calculation of coupling constants - C^{13}, P^{31} NMR, 2D-NMR spectra - Principle and applications.

Electron Spin Resonance Spectroscopy - Basic principles - Factors affecting "g" value - Hyperfine splitting - Deuterium, methyl, benzene, naphthalene, anthracene, xylene (o,m,p-), p-benzosemiquinone radicals - Calculation of electron density - McConnel equation - Fine structure in ESR - Zero field shifting and Kramer`s degeneracy - Double resonance – ELDOR and ENDOR - Study of unstable paramagnetic species - Spin labeling studies of bio-molecules.

References

1. Gurdeep Raj, Chemical Kinetics, Goel Publishing House.
2. FrostA.A and Pearson.R.G, Kinetics and Mechanism, Wiley Eastern, Pvt. Ltd.
3. Laidler.K.J, Chemical Kinetics, Third edition, New Delhi TATA McGrawHill Co. (1984).
4. Kuriacose and Rajaram, Kinetics and Mechanism of Chemical Transformation, Macmillan & Co, Delhi (1993).
5. Lee.J.F, Sears.F.W and Turcottee.D.L, Statistical Thermodynamics (1972)
6. Gupta.M.C, Statistical Thermodynamics, Wiley Easter Ltd., (1990)
7. Donald McQuarrie, Stastistical Thermodynamics, Indian Edition, Viva Books Private Ltd., New Delhi (2003).
8. Ferrell L Hill, Introduction to Statistical Thermodynamics, Addison-Wesley Publishing Company, INC, London (1962).
9. Kuriakose J C and Rajaram J C, Thermodynamics, Jalandar Shoban LalCo., (1996).
10. B. P. Straughan and S. Walker - Spectroscopy (vol. I).
11. Banwell C N, Molecular spectroscopy, New Delhi, TATA McGraw HillCo. (1997).
12. Drago R S, Physical Methods in Inorganic Chemistry, New Delhi, East West Press Ltd, (1971).
13. Chang R, Basic Principles of Spectroscopy, New Jersy, Englewood Cliffs(1978).
14. Straughan B P and Walker S, Spectroscopy Volume 1,2,3, New York, London Chapman and Hall, A Halstet Press Book, John Wiley & Sons Ins. (1975).
15. Barrow G M, Introduction to Molecular Spectroscopy, Tata McGraw Hill Edition (1993).
16. Gurdeep R Chatwal and Sham K Anand, Spectroscopy, Himalaya Publishing House (2009).
17. R. M. Silvertein and G. C. Basseler - Spectroscopic identification of organic compounds.

SEMESTER – III			
Core Elective - II Phytochemistry and Photochemistry			
Code : 17PCHE31	**Hrs / Week : 5**	**Hrs / Sem : 75**	**Credits : 5**

Unit I Biomolecules

Synthesis and reactions of oxazole, imidazole, coumarins, benzopyrazole and anthocyanins - synthesis of flavones - Pyranose and furanose forms of aldohexose and ketohexose - Methods used for the determination of ring size - Structural elucidation of maltose, sucrose and lactose - Starch and cellulose - Nucleic acids, nucleotides, polynucleotides and nucleosides.

Unit II Alkaloids and Terpnoids

Alkaloids – Introduction - General methods of extraction – Classification - Degradation studies - HEM, Emde and Von-Braun - Structural elucidation of papaverine, morphine and quinine, cocaine.

Terpenoids – Introduction - General methods to elucidate the structure of terepenes - Structural determination of camphor, zingiberine, α-pinene and squalene.

Unit III Steroids

Classification – Structural elucidation of cholesterol and ergosterol – Structural elucidation of androsterone, testosterone, progesterone and Oestrone.

Conversion of Cholesterol into androsterone, progesterone, testosterone, 5α- and 5β-Cholanic acid - Conversion of Oestrone to Oestriol.

Unit IV Photochemistry and Green Chemistry

Photochemistry - Basic principles - Jablonski diagram - Photosensitization - Photochemical reactions - Photoreduction – Photooxidation - Photochemical rearrangemen t- Norrish type I and II reactions - Paterno-Buchi reaction, Barton reaction and di- π methane rearrangement.

Green Chemistry - Twelve principles, atom economy- addition and rearrangement reaction, substitution reaction, elimination reaction - Green solvents - Supercritical CO_2, H_2O, Ionic liquids.

Unit V Pericyclic reactions

Atomic and molecular orbitals – Woodward-Hoffmann rules - FMO and MO correlation diagram approaches - Electrocyclic reactions - con and dis rotatory motions for 4n and 4n+2 system (butadiene and 1,3,5-hexatriene) - Stereochemical course of electrocyclic reaction in terms of conservation of orbital symmetry - Cycloaddition - suprafacial and antarafacial additions, [2+2] and [4+2] reactions (ethylene and butadiene) – Sigmatropic rearrangements - [i,j] shift of C-H and C-C bonds (1,3 1,5 and 3,3 system).

References

1. Finar I L, Organic Chemistry Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).
2. Gurdeep Chatwal, Organic Chemistry of Natural Products, Vol II, Himalaya Publishing House, Bombay, (2003).
3. Nasipuri D, Stereochemistry of Carbon Compounds, Second Edition, New-Age International Publishers, New Delhi (1996).
4. Ahluwalia, V. K and Rajender S. Varma, Green Solvents for Organic synthesis, Narosa Publishing House Pvt. Ltd. (2009).
5. Paul T Anastas, Text Book on Green Chemistry, OUP, (2006).

SEMESTER – III	
Self Study	**CHEMISTRY FOR NATIONAL ELIGIBILITYTEST - II**
Code : 17PCHSS2	**Credit : 1**

Inorganic Chemistry

1. Concepts of acids and bases, Hard-Soft acid base concept, Non-aqueous solvents.
2. Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds.
3. Transition elements and coordination compounds: reaction mechanisms.
4. Organometallics in homogeneous catalysis.
5. Cages and metal clusters.
6. Bioinorganic chemistry: photosystems, porphyrins, oxygen transport, electron- transfer reactions; nitrogen fixation.
7. Characterisation of inorganic compounds by NMR, EPR, NQR, and microscopic techniques.
8. Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

Organic Chemistry

1. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.
2. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.
3. Pericyclic reactions – electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.
4. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O,N,S).

5. Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids. Biogenesis of terpenoids and alkaloids.
6. Structure determination of organic compounds by IR, UV-Vis, ^{1}H & ^{13}C NMR and Mass spectroscopic techniques.

Physical Chemistry

1. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance.
2. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.
3. Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions.
4. Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis.
5. Solid state: Crystal structures; Bragg's law and applications; band structure of solids.

SEMESTER – IV			
Common Core - Nanoscience And Technology			
Code : 17PPCC41	**Hrs / Week : 6**	**Hrs / Sem : 90**	**Credits : 4**

Unit I Introduction

History of Nanotechnology - Nano structures - importance of nanomaterials - Synthesis of nanomaterials - Physical methods - Laser Ablation, Evaporation, Sputtering and solvated metal Dispersion - Chemical methods - Thermolysis, Sonochemical approach, reduction of metal ions by hydrogen and Methanol - Biosynthesis (Elementary idea only).

Unit II Preparation and characterisation

Structural characterisation (X-ray diffraction, Scanning Tunneling Microscopy, Atomic force microscopy) - Properties of nanomaterials (Optical, Electrical and magnetic properties) – Synthesis of semiconductor nanomaterials (Precipitation methods, Thermal decomposition of complex precursors) - Synthesis of Ceramic nanomaterials - Physical methods (Gas condensation and Laser methods) - Chemical method (Sol-gel synthesis).

Unit III- Carbon nanotube

Carbon nanotube - Carbon allotropes (Diamond, Graphite, Carbon nanotubes) - Types of Carbon nanotubes – Graphene sheet to single walled nanotube - Synthesis of carbon nanotubes (Electric arc - Discharge method, Laser method, Fluidised bed CVD method, Solar production of Carbon nanotubes) - Purification and properties of Carbon nanotubes – Fullerenes - Purification and properties of Fullerenes.

Unit IV Quantum well, Quantum wire and Quantum dots

Introduction - preparation of Quantum nanostructures - Fermi gas and Density of states – Calculation of the density of states in 1,2 and 3 dimension- Infrared detector -Quantum wire(Production, Structure, Use), Quantum dot - Fabrication Techniques - Application of Quantum dots – Quantum dot information storage, Infrared photodetectors, Lasers.

Unit V Magneto electronics and Applications of Nanotechnology

Magneto electronics: Nanocrystalline soft magnetic materials - Permanent magnetic materials -Theoritical background - Super para magnetism - Coulomb blockade - Single electron

transistor – Spintronics - Giant magneto resistance - Quantum Hall Effect - Fractional Quantum Hall Effect.

Applications of Nanotechnology:Chemistry and Environment - Energy applications of Nanotechnology - Information and Communication- Heavy industry - Consumer goods - Nano medicine - Medical applications of molecular nanotechnology (Nanorobots, Cell repair machines, nanonephrology).

Book for Study:

1. Nano Physics, Dr.Sr.Geraldin Jayam

Unit	**Book no.**	**Page No**
III	1	2.1-2.7,2.14-2.20,2.26-2.29
IV	1	4.1-4.10,4.15-4.30
V	1	5.1-5.5,5.10-5.30

Book for Reference

1. Shanmugam.S, Nanotechnology, MJP Publishers, Chennai(2011)
2. Parthasarathy. B.K, Nanostructure and Nanomaterials, Isha Books, Delhi(2007)
3. Fahrner.W.R (Ed), Nanotechnology and Nanoelectronics- materials, Devices, measurement techniques, Spinger(2004)
4. Charles.P. Poole Jr Frank J. Owens;John Wiley & Sons inc.Publication(2003)
5. Massimiliano Di ventra, Stephane Evoy, James R. Heflin Jr(Editors) , Introduction to Nanoscale science and Technology Springer(2009)
6. Guozhong Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press, London(2004).

SEMESTER – IV			
Core VIII Inorganic Chemistry - III			
Code : 17PCHC41	**Hrs / Week : 6**	**Hrs / Sem : 90**	**Credits : 4**

Unit I Inorganic photochemistry

Laws of photochemistry - Photo physical processes - Prompt and delayed reactions - d-d and charge-transfer reactions - bimolecular deactivation and energy transfer - Transitions in metal-metal bonded systems - Photo substitution - Photo aquation - Photo anation - Adamson's rules - Photo rearrangement - Photo redox reations - Photochemistry of Cr(III), Co(III), Rh(III) and Pt(II) complexes - Photochemistry of ruthenium polypyridyls - Photochemistry of organometallic compounds - Applications in semiconductor electrodes.

Unit II Bioinorganic Chemistry I

Metalloenzymes - Role of zinc - Zinc enzymes (Carboxypeptidase A, Carbonic anhydrase, alcohol dehydrogenase) - Xanthine oxidase, aldehyde oxidase, Acid phosphatases - Enzymes dealing with H_2O_2 and O_2 - Catalases, Peroxidases, Oxidases, Oxygenases (cytochrome P_{450}), Superoxide dismutase(Cu) –Chlorophyll and Vitamin B_{12} - Structure and mechanisms of action - Chelation therapy - Applications of complexes of Pt and Au in medicine.

Unit III Bioinorganic Chemistry II

Molecular mechanism of ion transport across membranes (Na and K ions) - Ionophores - Transport and storage of iron - Siderophores, Transferrin, Ferritin – Porphyrins - O_2 binding properties of heme (haemoglobin and myoglobin) and non-heme proteins (hemocyanin & hemerythrin) - their coordination geometry and electronic structure, co-operativity effect, Hill coefficient and Bohr effect - Electron transfer proteins - structure and functions of ferredoxin, rubidoxin and cytochromes and blue copper proteins – Photosynthesis - PS-I, PS-II, in vivo and in vitro nitrogen fixation.

Unit IV Inorganic chains, rings, cages and clusters

Homocyclic and hetrocyclic inorganic ring systems - Isopoly and heteropoly anions - Silicates, polysilicates and aluminosilicates, sulphur nitrides, borazines, Phosphazenes,

phosphazene polymers - Synthesis, properties and structure of boranes, [styx notation] heteroboranes, metalloboranes and metallo carboranes, silicones, metal - metal bonds - Clusters - carbonyl clusters, anionic and hydrido clusters, carbide clusters, sulphur metal clusters, Wade's rule - Isolobal relationships between main group and transition metal fragments.

Unit V Organometallic Chemistry

16 and 18 electron rules, synthesis, structure and bonding in mono and polynuclear metal carbonyls, nitrosyls, carbonylate ions, carbonyl hydride complexes, dinitrogen as ligands in organometallic compounds - Wade-Mingos-Lauher rules, Isolobal analogies IR of carbonyl coumpounds - Synthesis and reactivity of metal alkyls, carbenes, carbynes, carbides, alkenes, alkynes, and arene complexes - Metallocenes and bent metallocenes - Bonding in metallocenes.

References

1. James. E. Huheey , Ellen. A. Keiter and Richard. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, Harper Collins College Publishers, 4th Edition, 1993.
2. Shriver D.F., Atkins P.W. and Langford C.H., inorganic chemistry, ELBS, Oxford university Press, 1994.
3. Gary L. Miessler, Donald A. Tarr, Inorganic chemistry. Pearson Publications, third edition.
4. Catherine Housecroft, Alan G. Sharpe-Inorganic Chemistry (3rd Edition), Prentice Hall , 2007.
5. Albert Cotton. F, Geoffrey Wilkinson, Carlos. A. Manic and Manfred Bochman, Advanced Inorganic Chemistry, Wiley Interscience Publication , 6th edition, 1999.
6. Purcell K.F. and Kotz J.C, Advanced Inorganic Chemistry , Saunders Golden Publishers
7. Rohatgi Mukherjee K.K., Fundamentals of Photochemistry, New age international limited.
8. Gurdeep Raj, Advanced Inorganic chemistry II, Goel publishing house, Krishna prakashan media (P) Ltd.
9. Robert H. Crabtree, The Organometallic Chemistry Of The Transition Metals, John Wiley & Sons, Inc., Publication, 4th Edn.
10. Lee J.D., Concise Inorganic Chemistry, Blackwell Science Ltd., 5th Edition, Reprint 2003.

SEMESTER – IV			
	Core IX	Organic Chemistry - III	
Code : 17PCHC42	Hrs / Week : 6	Hrs / Sem : 90	Credits : 4

Unit I Spectroscopy I

UV – Visible and IR spectroscopy - Absorption laws - Types of electronic transitions – Instrumental and Sampling – Solvent effect – Application of Woodward- Fieser rule to calcualte λmax values of conjugated diene, triene, polyenes, α and β unsaturated carbonyl compounds - Optical rotatory dispersion and circular dichroism - Octant rule, α-haloketone rule and their applications.

IR spectroscopy – Instrumentation - Characteristics of IR absorption of different functional groups - Factors influencing vibrational frequencies - Hydrogen bonding - Inter and intra molecular hydrogen bonding.

Unit II Spectroscopy II

PMR spectroscopy - Basic principle - Number of signals - Chemical shift - Factors influencing chemical shift - Spin–spin coupling in AX, ABX type molecules - Geminal, vicinal and long range coupling - NOE in stereochemistry - FT-NMR - C^{13} NMR - 2D NMR – COSY – NOESY - INADEQUATE - DEPT - Broad and off resonance decoupling applications.

Unit III Spectroscopy III

Mass spectrometry - Instrumentation- Basic principles - Techniques of Ion production – EI, CI, FD, FAB, ESI-MS, MALDI-MS - Base peak - Molecular ion - Nitrogen rule - Metastable ion - Isotope ion - Daughter ion - Calculation of molecular formula - Fragmentation pattern of various classes of organic compounds - Hydrocarbons, alcohols, amines, aldehyde, ketone, ether, ester, acids and phenols - Mc-Lafferty rearrangement - Problems on combined applications of UV -Visible, IR, NMR and Mass spectrometric methods to structural elucidation of organic compounds.

Unit IV Conformational Analysis

Conformations of mono and disubstituted cyclohexanes - Effect of hydrogen bonding - Dipole and steric effects on the disubstituted cyclohexanes – Conformational analysis and

reactivity of acyclic and cyclic compounds (6 members) – Conformational analysis of decalin and perhydrophenanthrene - Curtin-Hammett principle.

Unit V Some typical reactions and applications in organic synthesis and Green Chemistry

C-C and C= C bond forming reactions - Acylation and alkylation - Mannich – Reimer-Tieman – Reformatsky – Ullmann - Storck Enamine – Shapiro - Wittig – Horner - Peterson, Heck - Mc.Murray reactions - Ring formation by Dieckmann, Acyloin condensation, Simmons-Smith reaction - Reduction and oxidation in synthesis - Catalytic, hydrogenation - Wolff-kishner, reduction - Oppenauer oxidation

Solid state and non solid state microwave assisted reaction – Stille reaction - suzuki reaction – Krohnka reaction – Fuyama reaction- sonogashira reaction.

References

1. Silverstein R M and Bassler G C, Spectrometric Identification of Organic Compounds, Fourth Edition, John- Wiley and Sons, New York (1993).
2. Ahluwalia V.K and Parshar R.K, Organic Reaction Mechanism Second Edition , Narosa Publishing House , 2005.
3. Finar I L, Organic Chemistry Volume I and II, Sixth Edition, ELBS with Longmann, Singapore (1997).
4. March J, Advanced Organic Chemistry, Fourth Edition, John-Wiley andSons, New York (1992).
5. Gurdeep Chatwal, Organic Chemistry of Natural Products, Vol II, Himalaya Publishing House, Bombay, (2003).
6. Nasipuri D, Stereochemistry of Carbon Compounds, Second Edition, New-Age International Publishers, New Delhi (1996).
7. P.S.Kalsi, Organic Reaction and their Mechanisms, New Age International, Third edition, (2011)
8. Warren S, A Programmed Synthon approach- John Wiley & Sons
9. Warren S, A Programmed Synthon approach- John Wiley & Sons
10. Ahluwalia, V. K and Rajender S. Varma, Green Solvents for Organic synthesis, Narosa Publishing House Pvt. Ltd. (2009).
11. Paul T Anastas, Text Book on Green Chemistry, OUP, (2006).

SEMESTER – III & IV			
INORGANIC PRACTICALS - II			
Code : 17PCHCR4	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Preparation of single stage inorganic complexes (a minimum of 6 complexes)

    1. cis potassiumdiaquadioxalatochromate(II) dihydrate
    2. trans potassiumdiaquadioxalatochromate(II) dihydrate
    3. tristhioureacopper(I)chloride dihydrate
    4. hexathiourealead(II)nitrate
    5. pentaamminenitritocobalt(III) nitrate
    6. hexaamminecobalt(III)chloride
    7. aquapentamminecobalt(III)chloride
    8. pentakisthioureadicopper(I) nitrate trihydrate

2. Quantitative estimation of a mixture containing two metal ions (Volumetric and Gravimetric estimations).
    1. Estimation of Cu^{2+} and Ni^{2+} ions.
    2. Estimation of Cu^{2+} and Zn^{2+} ions.
    3. Estimation of Fe^{2+} and Cu^{2+} ions.
    4. Estimation of Fe^{2+} and Ni^{2+} ions.
    5. Estimation of Ca^{2+} and Mg^{2+} ions.
    6. Estimation of Ca^{2+} and Ba^{2+} ions.

3. Analysis of ores and alloys (Course work only).

Note: For examination, a mixture may be given from which one cation is to be estimated volumetrically and the other gravimetrically.

References

1. Arthur I. Vogel, A Text book of Quantitative Chemical Analysis.
2. Mendtam. J et. al., Vogel's Text book of Quantitative Chemical Analysis, Pearson Education, 6^{th} edition.

SEMESTER – III & IV			
ORGANIC PRACTICALS - II			
Code : 17PCHCR5	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Quantitative Analysis

i) Estimation of ethyl methyl ketone

ii) Estimation of glucose-Lane Eynon method

iii) Estimation of glucose- Bertrand's method

iv) Determination of saponification value of oil.

v) Estimation of iodine value of oil.

2. Preparation of Organic compounds (Double stage)

i) Preparation of p-bromoaniline from acetanilide

ii) Preparation of m-nitrobenzoic acid from ethylbenzoate

iii) Preparation of p-nitro aniline from acetanilide

iv) Preparation of 1,3,5-tribromobenzene from aniline

v) Preparation of benzpinacolone from benzophenone

Note: Each student is expected to submit recrystallised samples of the preparation during her regular practical for evaluation during practical examinations.

3. Course work

i) Estimation of phenol

ii) Estimation of aniline.

iii) Estimation of Ascorbic acid

References

1. Vogel's Textbook of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, P.W.G.Smith, and A.R. Tatchell, V Edition, Pearson Education Ltd.,
2. Ganapragasm and Ramamurthy , Organic Chemistry Lab Manual, Second Edition, S.Vishwanathan Printers and Publishers (P) Ltd., Chennai
3. Ragupathi Mukhopadhyay, Pratul Chatterjee, Advanced Practcal Chemistry, Books and Allied (p) Ltd., Third edition, (2007)

SEMESTER – III & IV			
PHYSICAL PRACTICALS - II			
Code : 17PCHCR6	**Hrs / Week : 4**	**Hrs / Sem : 60**	**Credits : 4**

1. Potentiometry

1. Determination of solubility product of sparingly soluble salts.
2. Determination of dissociation constant of a weak acid.

2. Potentiometric titrations

a) Redox titrations

i) Fe^{2+} Vs $Cr_2O_7^{2-}$

ii) I^- Vs MnO_4^-

iii) Fe^{2+} Vs Ce^{2+}

b) Precipitation titrations

i) Cl^- Vs $AgNO_3$

ii) I- Vs $AgNO_3$

iii) Mixture of Cl^- and I- Vs $AgNO_3$

3. Spectroscopy

Verification of Beer-Lambert's law. Determination of $[Mn^{2+}]$ and $[Cr^{3+}]$ by using UV-Visible spectrophotometer.

4. Adsorption:

Adsorption of acetic acid / oxalic acid on activated charcoal - Verification of Freundlich isotherm - Determination of unknown concentration.

5. Conductivity method

Study of Kinetics of ester hydrolysis and comparison of acid strength by conductivity method.

References

1. Viswanathan.B and Raghavan.P.S, Practical Physical Chemistry, Viva Books Pvt.LTD., (2005)
2. Michell.J.Sienko, Robert.A, Plane, Stanley.T. Martu, Experimental Chemistry, International student edition (`1984)
3. David. P. Shoemaker, Carl. W. Garland and Joseph.W.Nibler, Experiments in Physical Chemistry, McGraw Hill International edition
4. Levitt.B.P , Findlay's Practical Physical Chemistry, Edition IX
5. Yadav. J.P , Physical Chemistry Practicals
6. Peter Mathews.G , Experimental Physical Chemistry , Clarendan Press Oxford (1985).