MANONMANIAM SUNDARANAR UNIVERSITY
TIRUNELVELI
PG - COURSES – AFFILIATED COLLEGES
Course Structure for M.Sc. Chemistry
(Choice Based Credit System)
(with effect from the academic year 2016- 2017 onwards)
(44th SCAA meeting held on 30.05.2016)

Sem	Sub No.	Subject status	Subject Title	Hrs/ week	Cre-dits	Marks				
						Maximum			Passing Minimum	
						Int.	Ext	Tot.	Ext.	Tot
III	13	Core - 7	Organic Chemistry -III	5	5	25	75	100	38	50
	14	Core - 8	Inorganic Chemistry- III	5	5	25	75	100	38	50
	15	Core - 9	Physical Chemistry -III	5	5	25	75	100	38	50
	16	Core – 10	Scientific Research Methodology	3	3	25	75	100	38	50
IV	17	Core - 11	Organic Chemistry- IV	5	5	25	75	100	38	50
	18	Core - 12	Inorganic Chemistry -IV	5	5	25	75	100	38	50
	19	Core - 13	Physical Chemistry -IV	5	5	25	75	100	38	50
	20	Practical – IV	Organic Chemistry – II	4	4	50	50	100	25	50
	21	Practical – V	Inorganic Chemistry – II	4	4	50	50	100	25	50
	22	Practical -- VI	Physical Chemistry – II	4	4	50	50	100	25	50
	23	Project	Project work and viva-voce	3	3	50	50	100	25	50

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Organic Chemistry – III

UNIT-I : ALIPHATIC NUCLEOPHILIC SUBSTITUTION AND ELIMINATION REACTIONS:

Aliphatic Nucleophilic Substitution : Mechanism of S_N1, S_N2, S_Ni, S_N1', S_N2' and S_Ni' reactions- Effect of substrate, nucleophile, leaving group and solvent on the rate of substitution- Ambident nucleophile- NGP- Mechanism of esterifications and ester hydrolysis ($B_{AC}2$ and $A_{AC}2$ mechanisms only).

Elimination Reaction: E_1, E_2 and E_1CB mechanisms- Factors influencing elimination reactions- Hofmann and Satyzeff rules- Pyrolytic elimination- Chugaev and cope reactions- competition between substitution and elimination reactions.

UNIT – II: NMR SPECTROSCOPY

H^1NMR spectroscopy: Basic Principle – number of signals – chemical shift – Factors influencing chemical shift - spin–spin splitting– classification of spin systems – analysis of AX, AMX and ABX systems – Geminal, Vicinal and long range couplings–NOE in stereochemistry – FTNMR.

C-13 spectroscopy: Principle of proton decoupled C-13 spectroscopy - comparison with H^1NMR – chemical shifts (aliphatic, olefinic, alkynic, aromatic and carbonyl compounds).

2D NMR spectroscopy: H^1–H^1COSY, H^1–C^{13} COSY, NOESY, DEPT and INADEQUATE spectra.

UNIT – III: MASS SPECTROSCOPY

Basic Principles– Base peak – molecular ion – nitrogen rule – metastable ions – isotopic peak - daughter ions – Mc–Lafferty rearrangement – RDA – General rules for fragmentation pattern – Fragmentation pattern of simple compounds of hydrocarbons, alcohols, amines, aldehyde, ketone, ether, acids, phenols ,nitro compounds, alicyclic compounds .

Alternative electron impact ionization technique– CI, FAB, ESI – MS, MALDI –MS, MALDI-TOF, ICP- MS.

One conjunction problem based on UV, IR, H^1 NMR, ^{13}C NMR and Mass spectroscopic techniques is compulsory under section – c. Problems shall be based on the reference books.

UNIT-IV : ORGANIC PHOTOCHEMISTRY AND PERICYCLIC REACTIONS

Organic photochemistry: Jablonskii diagrams-intersystem crossing-energy transfer process-Photosensitization- alpha cleavage or Norris type-I and gamma hydrogen transfer or Norrish Type II cleavage – Paterno-Buchi reactions- Barton reaction, photo oxidation and reduction reaction - cis-trans isomerisation. - Di-π methane rearrangement.

pericyclic reactions: Atomic and molecular orbital's -Woodward-Hoffmann rules, FMO method and correlation diagram approaches:

Electrocyclic reaction: con and dis rotatory motions for 4n and 4n+2system (butadiene and 1,3,5-hexatrienes)- Stereochemical course of electro cyclic reaction in terms of conservation of orbital symmetry.

Cyclo addition: suprafacial and antarafacial, [2+2] and [4+2] cyclo addition reactions (ethylene and butadiene)

Sigmatropic rearrangements - [i, j] shift of C-H and C-C bonds (1,3) and (1,5) carbon migration.

UNIT-V : HETEROCYCLIC AND BIOMOLECULES

Synthesis and reactions of indole, oxazole, imidazole, thiazole, Carbazole, chromans, Chromons, pyrimidine, pyridazine, pyrazine, coumarins, benzopyrones and anthocyanins-synthesis of flavones, isoflavones, flavonol, and quercetin -Biosynthesis of flavonoids. Synthesis

Pyranose and furanose forms of aldohexose and ketohexose-methods used for the determination of ring size-A Detailed study on the structure of maltose, lactose and starch.

REFERENCES :

1. J.March, ' Advanced organic chemistry', Fourth Edition, John Wiley and Sons, Newyork, 2006.
2. Depuy, E.C.H. and Chapman, O.S., "Molecular reactions and photochemistry" , Prentice Hall, New York, 1988.
3. I.L. Finar, 'Organic Chemistry', volume 2, sixth Edition, Pearson Education Inc., Singapore, 2006.
4. Raj K. Bansal, 'Organic Reaction mechanisms", Tata Mc Graw Hill, Third Editon, 2007.
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6. S. Kalsi, 'Spectroscopy of organic spectroscopy', second Edition , New Age International publishers Limited, 1995 .

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10. D.H.Williams and Ian Fleming, 'Spectroscopic methods in organic chemistry,'fifth Editon, Tata Mc Graw Hill, 1988.
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14. Pavia, Lampmann, Kriz and Vyuyan, spectroscopy, cengage learning India Private Ltd., First Indian Reprint,2008.
15. D.H. William and R.D. Bower, 'Mass spectrometry – principles and Applications,' I. Howe, Mc Graw Hill.
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17.Singh, J., and Singh, J., "Photochemistry and Pericyclic reaction", New Age International, New Delhi, 2004.
18.H.O. House, 'Modern synthetic Reaction,'Second Edition , W.A. Benjamin, Inc., London, 1972
19.R.K. Mackie, M.M. Smith and R.A. Aitken,'Guide Book to Organic Synthesis' Second Edition, Longman Seientific and Technical, Singapore, 1990.
20.Carrutherus , W., " Some Modern Methods in Organic Syntheis", Third edition, Cambridge University Press, New York, 1997.
21.F.A. Carey and J.Sundberg,'Advanced Organic chemistry ' part A and B, Plenum Press, 2005.
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32. Bansal, K., "Heterocyclic Chemistry", Fourth edition, New Age International, New Delhi, 2005.
33. Organic chemistry by Clayden,Greeves, Warren & Wothers.
34. Pericyclic reactions by Ian Fleming.
35.Organic chemistry by John McMurry.
36. Organic chemistry by L.G. Wade. JR.
37. Named Organic reactions by Thomas laue & Andreas Plagens.

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Inorganic Chemistry - III

UNIT – I : ORGANOMETALLIC CHEMISTRY - I

Definition - 18 e^- and 16 e^-rules and its correlation to stability - Synthesis and structures of metal carbonyls, metal nitrosyls and dinitrogen complexes- Substitution reactions of metal carbonyls - IR spectral applications– identifications of bridging and terminal CO groups –-Stretching mode analysis of metal carbonyls–evidence for M-M bonds. Synthesis, properties and structural features of metal complexes with alkene, alkyne, allyl and arene systems. Metallocenes - synthesis, properties, structure and bonding with particular reference to ferrocene and berryllocene- covalent versus ionic bonding in beryllocene.Template synthesis of macro cyclic ligands.

UNIT - II : ORGANOMETALLIC CHEMISTRY- II

Organometallic compounds as catalysts and the requirements - Oxidative addition and reductive elimination- insertion and elimination reactions - nucleophilic and electrophilic attack of coordinating ligands - addition to bimetallic species and cyclo metallation reactions. Homogeneous catalysis –Wilkinson's catalyst and hydrogenation reactions, Tollman's catalytic loop; hydroformylation (oxo) reaction, Wacker and Monsanto acetic acid processes. Cluster compound, polymer-supported and phase-transfer catalysis. Heterogeneous catalysis – synthesis gas and water gas shift reactions; Fischer Tropsch process and synthetic gasoline, Ziegler-Natta polymerization and mechanism of stereo regular polymer synthesis. Cyclo oligomerisation of acetylenes (Reppe's or Wilke's catalyst)-Olefin isomerisation using Ni catalyst – olefin Meta thesis catalysed by Schröck type carbene.

UNIT- III : SPECTRAL METHODS TO THE STUDY OF INORGANIC COMPOUNDS– I

NMR Spectroscopy: ^{31}P, ^{19}F and ^{15}N - NMR - applications in structural problems based on number of signals, multiplicity, anisotropy (like $[H\ Ni(PPh_3)_4]^+$, $CFCl_3$, SF_4, TiF_4,PF_5, HPF_2, H_2PF_3, $PF_3(NH_2)_2$, P_4S_3, mer - and fac – Rh $(PPh_3)_3Cl_3$, $P_3N_3(CH_3)_2Cl_4$,$P_4N_4Cl_6(NHC_6H_5)_2$,NF_3, NH_3- fluxional molecules (including organometallic compounds) and study of fluxionality by NMR technique - NMR of paramagnetic molecules - contact shifts. Evaluation of rate constants - monitoring the course of reaction using NMR.

EPR spectroscopy: Zero field splitting and Kramer's degeneracy - Application of EPR in the study of transition metal complexes based on number of signals, multiplicity, anisotropy (like bis (salicylaldimine)copper(II),$[Cu(bpy)_3]^{2+}$,$[Cu(Phen)Cl_2]$,$[(NH_3)_5Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$,$Co_3(CO)_9Rh$, $[CoF_6]^{4-}$, $[CrF_6]^{3-}$, $VO(acac)_2$, $Fe(CO)_5^+$, $Fe(CO)_5^-$, $[Fe(CN)_5NO]^{2-}$,$[Mn(dppe)_2]$,$[MnF_6]^{4-}$). Applications in predicting the covalent character of M-L bond and Jahn-Teller distortion in Cu(II) complexes. EPR spectroscopy of metallo biomolecules: copper and iron proteins.

UNIT – IV : THERMOANALYTICAL AND SPECTROANALYTICAL METHODS

Theory and principles of thermo gravimetric analysis, differential thermal analysis and differential scanning colorimetry – characteristic features of TGA and DTA curves-factors affecting TGA and DTA curves- complementary nature of TGA and DTA – applications of thermal methods in analytical chemistry - thermometric titrations - the study of minerals and metal compounds. Principle and applications of colorimetry, spectrophotometry, nephelometry, turbidimetry, fluorimetry, atomic absorption spectroscopy and atomic emission spectroscopy based on plasma sources.

UNIT -V : INORGANIC PHOTOCHEMISTRY

Frank Condon and thermally equilibrated excited (THEXI) states - properties of excited states of metal complexes (life time, redox potential etc.) – charge transfer excitation – bimolecular deactivation (quenching) and energy transfer – photochemical path ways : oxidation-reduction, isomerisation and substitutional processes – photochemistry of Cr(III), Co(III) complexes – Photochemical reactions of metal carbonyls. Photo physical and photochemical properties of $[Ru(bpy)_3]^{2+}$and comparison with $[Fe(bpy)_3]^{2+}$– Applications of inorganic photochemistry: photochemical conversion and storage of solar energy – inorganic photochemistry at semi-conductor electrodes - Catalyzed photo reduction of CO_2 and CO – TiO_2as a green photo catalyst in removing air and water pollutants.

REFERENCES:

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19. V. Balzani and A. Juris, *Coord. Chem. Rev*., 211, 97–115, 2001.
20. Inorganic chemistry by Catherine E. Housecroft.
21. Inorganic chemistry by Miessler.
22. NMR, NQR, EPR & MOSSBAUER spectroscopy in inorganic chemistry by R.V.Parish.
23. Biological inorganic chemistry: An introduction by Robert R.Chrichton.
24. Bioinorganic chemistry: A short course by Rosette M. Roat – Malone.
25. The Organometallic chemistry of the transition metals by Robert H. Crabtree.

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Physical Chemistry- III

UNIT-I : GROUP THEORY I Symmetry elements and operations. Groups-Types of groups abelian, non-abelian cyclic and sub-groups. Similarity transformations and classes of symmetry operations. Point groups and Schoenflies symbols. Representation of groups-Matrix representation of symmetry operations-reducible and irreducible representations. Direct product representation. Rearrangement theorem. Construction of multiplication tables for C_{2v}, C_{3v} and $C_{2h.}$ The Great Orthogonality theorem and its consequences-Character table - construction of character tables for C_{2V}, C_{3V}, C_{4V}, C_{2h}, and D_2 point groups.

UNIT-II: GROUP THEORY II Standard Reduction Formula. Symmetry selection rules for infrared, Raman and electronic Spectra and Mutual exclusion principle. Determining Symmetries of normal vibrational modes for non linear molecules H_2O, NH_3 and trans-N_2F_2. Projection operators and construction of Symmetry Adopted Linear Combinations. Determination of Hybrid orbitals in non-linear molecules (BF_3, CH_4, XeF_4, BF_3, PF_5, and SF_6). Electronic Spectra of Ethylene and formaldehyde- Simplification of HMO calculations using group theory. Calculation of delocalization energy for ethylene, cyclo propenyl, 1,3-butadiene, and benzene systems.

UNIT- III : NQR AND MOSSBAUER SPECTROSCOPY

Principle of NQR spectroscopy - nuclear charge distribution and quadrupole moment. Quadrupole nucleus and its interaction with electric field gradient, nuclear orientations, the asymmetry parameter, quadrupole transitions in spherical and axially symmetric fields, quadrupole energy levels and field gradient. NQR spectra-effect of magnetic field on the spectra, relationship between electric field gradient and molecular structure.

Mössbauer spectra-Principles and experimental technique- sources, absorber, calibration. Doppler shift, recoil energy, isomer shift, quadrupole splitting, magnetic hyperfine interaction, Chemical applications- Quadrupole splitting in iron complexes.

UNIT – IV: MAGNETIC RESONANCE SPECTROSCOPY (NMR AND EPR)

Theory of NMR spectroscopy: nuclear spin and magnetic nuclei, nuclear magnetic moment, behavior of a bar magnet in a magnetic field, the NMR transitions, the Bloch equations, relaxation mechanisms. Parameters of NMR: measuring the chemical shift, shielding and deshielding of magnetic nucleus, chemical shifts in aliphatic and aromatic compounds, factors affecting chemical shift-inductive effect, anisotropy of chemical bonds , hydrogen-bond, temperature, solvent. Spin-spin splitting : effect of spin-spin splitting on the spectrum, mechanism of spin-spin splitting, chemical exchange, coupling constants; application of spin-spin splitting to structure determination- geminal- vicinal- long-range coupling; factors influencing geminal and vicinal coupling. ^{13}C, ^{19}F, ^{31}P NMR-range of chemical shift values, spectra of typical examples.

Electron paramagnetic resonance spectroscopy: theory of EPR spectroscopy, presentation of the spectrum, nuclear hyperfine splitting in isotropic systems. EPR spectra of anisotropic systems: anisotropy in g- values causes of anisotropy, anisotropy in hyperfine coupling, EPR spectra of triplet states and zero field splitting.

UNIT-V : ELECTRONIC SPECTROSCOPY

Electronic spectra of molecules: Born-Oppenheimer approximation, Franck-Condon Principle, selection rules, intensity of electronic transition, Vibronic coupling, types of electronic transitions. Chemical analysis by electronic spectroscopy: assignment of electronic transitions, application to the study of organic compounds. Emission spectroscopy: state of electronically excited molecules- dissociation, reemission, emission spectra of molecules.

Photo electron spectroscopy (PES): principle and technique of PES, ultra violet PES, X-ray PES. Lasers: nature of stimulated emission-coherence and mono chromaticity, population inversion, cavity and mode characteristics, Q-switching, mode locking; types of lasers-solid-state, gas, chemical, and dye lasers

REFERENCES:

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2. F. Albert Cotton, Chemical Applications of Group Theory,Third Edition, John Wiley & Sons, Singapore, 2003.
3.V. Ramakrishnan and M. S. Gopinathan,Group Theory in Chemistry, Vishal Publication,1986.
4. Robert L. Carter, Molecular Symmetry and Group Theory, John Wiley and Sons, Inc., New York, 1998.
5. R.L. Flurry, Jr, Symmetry Groups – Prentice Hall, New Jersy 1980.
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8. B.K. Battacharya,Group Theory and its Chemical applications
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Scientific - Research Methodology

Unit – I: LITERATURE SURVEY

Source of chemical information – primary, secondary, tertiary sources-literature survey-Indexes and abstracts in science and technology – Applied science and technology index, chemical abstracts, chemical titles, current chemical reactions, current contents and science citation index.

Classical and comprehensive reference works in chemistry-synthetic methods and techniques, treatises, reviews, patents and monographs.

UNIT - II : CHEMICAL ABSTRACTS:

Current awareness searching: CA weekly issues, CA issue indexes.

Retrospective searching: CA volume indexes-general subject index, chemical substance index-formula index, index of ring systems, author index, patent index.

CA collective indexes: collective index (CI), decennial index (DI)

Access points for searching CA indexes- Index guide, general subject, terms, chemical substance names, molecular formulas, ring systems, author names, patent numbers.

Locating the reference: finding the abstract, finding the original document chemical abstract - service source index.

UNIT –III: CHOOSING A RESEARCH PROBLEM AND SCIENTIFIC WRITING

Identification of research problem – assessing the status of the problem - guidance from the supervisor – actual investigation and analysis of experimental results – conclusions.

Scientific writing-research reports, thesis, journal articles and books.

Steps to publishing a scientific article in a journal – types of publications-communications, articles, reviews, when to publish, where to publish, specific format required for submission.

Documenting- Abstracts-indicative (or) descriptive abstracts, informative abstract, footnotes, end notes, referencing styles-bibliography-journal abbreviations (CASSI), abbreviation used in scientific writing.

UNIT –IV: INSTRUMENTAL CHARACTERIZATION AND DATA ANALYSIS

Sample preparation of UV, FT-IR, TEM, SEM, EDAX, AFM and XRD techniques - Characterization of observed results – Data analysis - Report.

Errors in chemical analysis – classification of errors – determination of accuracy of methods – improving accuracy of analysis – significant figures – mean, standard deviation – comparison of results : "t" test, "f" test, Q test and "chi" square test – rejection of results – presentation of data.

UNIT –V: COMPUTER SEARCHES AND LITERATURE.

ASAP – Alerts, CA Alerts, scifinder, chemport, science direct, STN international, journal home pages. Online browsing of research articles – online submission of research papers in various Journals (ACS, RSC, Elsevier, Springer etc.) –Instructions to the authors – Impact factors. Writing project proposal to funding agencies (UGC, DST etc.).

REFERENCES

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3. R.O.Bullet, Preparing thesis and other manuscripts.
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18. B.K.Sharma, Instrumental methods of chemical analysis.
19. D.A. Skoog and M.West, Fundamentals of analytical chemistry.
20. J.D.Dick, Analytical chemistry.
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Organic Chemistry – IV

UNIT-I: REACTION UNDER INTERMEDIATE CHEMISTRY

Reaction under Carbanion Intermediate: Clasien, Knoevenegal, Stobbe, Darzen, acyloin condensation Shapiro reaction and Julia olefination.

Reaction through carbene intermediate: Bamford – Stevens and simmons-smith reactions

Reaction under Carbocation intermediate: Oxymercuration, halolactonisation, Baeyer-villiger oxidation

Reaction following Radical intermediate: Mc Murray coupling, Gomberg-Pechmann and Pschorr reactions.

Reaction involving Ylide intermediate: Wittig reaction and Peterson olefination.

UNIT-II: CONFORMATIONAL ANALYSIS

Conformation and configuration-conformational free energy-conformational analysis of mono substituted (alkyl, halogens) and 1,1-disubstituted (alkyl) and 1,2-1,3-and 1,4-dimethyl substituted cyclohexanes -compounds existing in boat form-conformation of cyclohexanone, decalin and perhydrophenanthrene-curtin-Hammett principle- conformation and reactivity of acyclic and cyclic compounds (6membered).

UNIT-III: RETEROSYNTHETIC 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, Baclofen, phenanthrene , Trihexyl phenydyl, S-propanediol, R and S – Epichlorohydrin, Abietic acid, Isonootkatone, cascarillic acid, camphor and 2,4-dimethyl-2-hydroxy pentanoic acid.

UNIT-IV: REAGENTS IN ORGANIC SYNTHESIS

2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), DMSO, Super hydrides- Dess-martin-periodinane-Osmium tetra oxide.

Modern Reagents: Introductory treatment of the application of silicon (Tri alkyl silyl halides, organo silanes), Boron (9 – BBN, borane, and alkyl borane), phosphorus (phosphoranes), palladium (Still coupling, Suzuki Coupling, Heck and Negishi reactions) samarium(SmI_2),Ruthenium(RuO_2,Ru-Binap Complex), Rhodium(Wilkinson's Catalyst), and platinum (PtO_2, Adam's Catalyst) reagents in organic synthesis.

UNIT-V: STEROID

Classification- structural elucidation of cholesterol, irradiated products of ergosterol. Conversion of cholesterol to androsterone, progesterone, testosterone, 5α- and 5 β-cholanic acids. Conversion of Oestrone to Oestriol, Oestrodiol and vice-versa. Structural elucidation of equilenin (synthesis not expected). Conformational structure of cholestane and Coprostane. General study of Bile acids and Prostaglandins.

REFERENCES :

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2. R.T. Morrison and R.N. Boyd,'Organic Chemistry' sixth Edition, Prentice Hall, 1994
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Inorganic Chemistry- IV

UNIT - I : SPECTRAL METHODS TO THE STUDY OF INORGANIC COMPOUNDS – II

Mossbauer spectroscopy: Principle – isomer shift (IS) – splitting of resonance lines: quadrupole splitting and magnetic hyperfine splitting. Applications: MB spectra of iron compounds/ complexes – structural elucidation, π- bonding effect, HS and LS determination, spin state crossover determination, cis–trans determination – nature of the complexes - mixed valence complexes. Tin compounds: MB spectra of Sn(II) and Sn(IV) compounds, oxidation states of Sn in its different compounds. MB spectra of iodine and ^{129}Xe containing compounds.

ORD AND CD - Optical isomerism in octahedral complexes– absolute configuration of chelate complexes from ORD and CD.

UNIT - II: SPECTRAL METHODS TO THE STUDY OF INORGANIC COMPOUNDS – III

Photo electron spectroscopy : Theory – types of PES –origin of fine structures – shapes of vibrational fine structures – adiabatic and vertical transitions – PE spectra of homo (like N_2, O_2) and hetero nuclear diatomic molecules (like CO) - polyatomic molecules like H_2O, CO_2, CH_4,NH_3.Evaluation of vibrational constants – Koopman's theorem - application and limitation of the theorem. XPS (ESCA): structure of N_3^-ion, CCl_3CH_3, N(1s) spectrum of $[Co(en)_2(NO)_2]NO_3$,C(1s) spectrum of $C_2H_5COOCF_3$.Shake-up and shake-off processes – Structural and bonding information in metal carbonyls – Auger (OhJay) electron spectroscopy.

NQR spectroscopy - Applications of NQR spectroscopy -finger print technique. Investigating the electronic structure of molecules - information about EFG of nuclei - ionic character and hybridization of the bonds - structure of change transfer complexes - Phase transition - hydrogen bonding.

UNIT III –BIOINORGANIC CHEMISTRY- I

Non-metals and metals in biological systems, essential and trace elements; classification of metallo-biomolecules, coordination environment and entatic state. Metallo porphyrins– chlorophyll and photo synthesis; cytochromes, hemoglobin, myoglobin and dioxygen binding, vitamin B_{12} and co-enzyme - *in vivo* and *in vitro* nitrogen fixation. Iron storage and transport: ferritin, transferrins and siderophores - iron proteins: hemerythrin, cytochrome P450 enzyme, ferredoxin and rubredoxin.

UNIT - IV: BIOINORGANIC CHEMISTRY - II

Copper proteins and Enzymes: plastocyanin, azurin, hemocyanin and ascorbic oxidase - different types of Cu present in proteins and enzymes. Zinc enzymes: carboxypeptidase A, carbonic anhydrase and superoxide dismutase. Inhibition and poisoning of enzymes illustrated by xanthine oxidase and aldehyde oxidase. Toxicity of metals and the role of metallothionins - excess and deficient levels of Cu and Fe and the consequent diseases - chelate therapy – metal complexes as drugs, anticancer and antiarthritic agents. Metal complexes as probes of nucleic acids.

UNIT – V: CHEMISTRY OF INORGANIC MATERIALS

Synthesis of inorganic materials – high temperature reactions and experimental methods – precipitation, gel, solution and hydrothermal methods, synthesis in sealed tubes and special atmospheres. Low temperature methods. Insertion compounds of metal oxides – Intercalation compounds of graphite and transition metal disulphides. Zeolites: structures and properties – pillared clays – fullerenes and fullerides.

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Physical Chemistry- IV

UNIT-I: CHEMICAL KINETICS I

Potential Energy surfaces-energy of activation. Thermodynamic treatment-statistical mechanism and chemical equilibrium- Kinetics of some reactions. Theories of reaction rates: Collision theory-steric factor. Absolute Reaction Rate Theory (ARRT)-derivation of rate equations and application of ARRT to bimolecular processes. Comparison between collision and Absolute Reaction Rate theories. Unimolecular reactions; Lindemann - Christiansen hypothesis, Hinshelwood, RRK, RRKM and Slater theories. Rate expressions for opposing, parallel and consecutive reactions. Chain reactions and its characteristics-steady state treatment, kinetics of H_2-Br_2 reactions, formation of Phosgene-decomposition of N_2O_5. Rice-Herzfeld mechanism, Explosive reactions: H_2-O_2 reaction.

UNIT-II : CHEMICAL KINETICS - II

Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Brønsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation. Fast reaction kinetics- Flow techniques - relaxation theory and relaxation techniques - Temperature, Pressure, electric field and magnetic field jump methods; Flash photolysis and pulse radiolysis. NMR and ESR methods of studying fast reactions.

UNIT-III : SURFACE CHEMISTRY & CATALYSIS

Introduction: Adsorption- Physisorption and chemisorptions. Adsorption isotherms: Freundlich, Langmuir, BET and Gibbs adsorption isotherms. Surface area dertermination. ARRT to surface reactions. Micelles: Micelles and reverse micelles- micro emulsion-solubilisation.

Catalysis: Homogeneous catalysis- acid-base catalysis- van't Hoff and Arrhenius complexes for protropic and protolytic mechanisms. Bronsted catalysis law- Hammett acidity function. Heterogeneous catalysis. Chemical reactions on solid surfaces. Enzyme catalysis: Michaelis - Menton kinetics- Rate of enzyme catalyzed reaction- effect of substrate concentration, pH and temperature on enzyme catalyzed reactions.

UNIT-IV: POLYMER CHEMISTRY Polymers – definition – types of polymers – liquid crystalline polymers. Molecular mass- number and mass average molecular mass – determination of molecular mass (osmometry, viscosity, diffusion, light scattering, and sedimentation methods). Visco-elasticity, Rubber elasticity. Kinetics and mechanism of linear stepwise polymerization – addition polymerization – free radical, cationic and anionic polymerization. Kinetics of co-polymerization. Polymerization in homogeneous and heterogeneous systems. Stereochemistry and mechanism of polymerization.

UNIT-V: PHOTOCHEMISTRY AND RADIATION CHEMISTRY:

Photochemistry- Introduction. Laws of photochemistry, Quantum yield and its determination. Physical properties of electronically excited molecules: excited state dipole moment, acidity constant and redox Potentials. Photo physical processes in electronically excited molecules: Jablonskii diagram – Intersystem system crossing internal conversion, fluorescence, phosphorescence and other deactivation processes. Photo sensitization chemiluminescence and bioluminescence-Stern-Volmer equation and its applications – mechanisms of quenching – electron transfer – energy transfer–experimental techniques in photochemistry –chemical actinometers.

Radiation Chemistry-Differences between radiation chemistry and photochemistry – sources of high energy radiation and interaction with matter – radiolysis of water, solvated electrons – Definition of G-value- Dosimetry and dosimeters in radiation chemistry- applications of radiation chemistry in industries and biology.

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Organic Chemistry Practical

- Estimations, two stage preparations and chromatographic techniques have been included as the practical components.
- Microscale preparations are recommended for the simple reason, they are both economic-friendly and eco-friendly

A. List of Estimations

1. Ethyl methyl ketone
2. Glucose-Lane Eynon and method
3. Glucose-Bertrand's method
4. Saponification value of oil
5. Iodine value of oil
6. Determination of Percentage purity in an unsaturated acid.
7. Purity of Glucose

B. List of Two stage preparations

1. Benzaldehyde ⟶ Benzoic acid ⟶ m-nitro benzoic acid
2. Acetanilide ⟶ p-acetanilide ⟶ p-Bromoaniline
3. Methyl benzoate ⟶ m-nitro methyl benzoate ⟶ m-nitro benzoic acid
4. Acetanilide ⟶ p-nitro acetanilide ⟶ p- nitroaniline
5. Benzophenone ⟶ Benzo phenone oxime ⟶ Benzanilide
6. Benzophenone ⟶ Benzpinacol ⟶ Benzpinacolone
7. Phthalic acid ⟶ Phthalic anhydride ⟶ Phthalimide
8. Thiourea ⟶ s-benzyl isothiuronium chloride s-Benzyl-isothiuronium benzoate
9. Aniline ⟶ Tri bromoaniline ⟶ Sym-Tribromobenzene

Students are expected to submit at the time of practical examination at least eight recrystallised samples of the final products, for evaluation by the examiners.

C. For Class Work Only

(I)Chromatographic techniques

1. TLC of Nitroaniline
2. TLC of Analgesic Drug
3. Column Chromatography-Separation of leaf pigments
4. Paper Chromatography-Analysis of Inks and Dyes

(II)Spectral analysis:

5. Interpretation of H^1 NMR spectra of pure ethyl alcohol and aqueous ethyl alcohol.
6. DEPT spectra of isopentyl acetate.
7. Mass spectrum of Anisole, Phenol and Crotonaldehyde

N.B: 1.Section -C is course work only.

2. It is for the purpose of internal assessment only.

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Practical-V

Inorganic Chemistry Practical

I . 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 .

7. 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 .

II . Preparation of single stage inorganic complexes (a minimum of 10 complexes).

Note : Characterisation of any two metal complex prepared during the practicals by UV or IR spectral techniques (course work only)

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Practical- VI

Physical Chemistry Practical

I. **Potentiometric titrations**-

(a) Acid alkali titrations.

(b) Precipitation titrations (a) Mixture of Cl^- and I^- vs Ag^+

(c) Redox titrations (a) Fe^{2+} vs $Cr_2O_7^{2-}$
(b) Fe^{2+} vs Ce^{4+}
(c) I^- vs $KMnO_4$

(d) Determination of dissociation constant of weak acids.

(e) Determination of solubility product of sparingly soluble silver salts.

(f) Determination of activity and activity coefficient of ions.

(g) Determination of pH of a buffer solution using a quin hydrone electrode.

II. Titration using pH meter

(a) Determination of dissociation constant of dibasic acid.

III. Freundlich Adsorption isotherm

(a) Adsorption of oxalic acid/acetic acid on charcoal.

IV. Kinetic studies

(a) Kinetics –acid hydrolysis of ester –comparison of strength of acids.
(b) Kinetics –Persulfate –Iodide –clock reaction-primary salt effect.

REFERENCES: (Practical I and II)

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Project work and viva – voce