Department of Chemistry, Kakatiya University introduces Choice Based Credit System (CBCS) for M.Sc. (2 Year course) chemistry for the students admitted in M.Sc. Chemistry course from 2016-17 academic year onwards.

Scheme for CBCS, the workload for each paper, distribution of marks, the number of credits and scheme of examination are attached herewith.

Internal Assessment examination will be conducted twice in every Semester. The main examination (theory and practical) will be conducted at the end of each semester.

One open elective in III semester and one is in IV semester are offered by Department of Chemistry for all the PG-students.

Students joined in M.Sc. Chemistry should choose one open elective offered by Department of chemistry or any other Department of Kakatiya University.

The syllabi of theory and practical papers of I, II III, and IV semesters are enclosed. The syllabi of open elective offered in IV semester will be kept available for the next academic year.

– Prof. Gade Dayakar
Chairperson
Board of Studies in Chemistry
### Curriculum Scheme of Examination

#### Semester – I

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Seminar

Total | 38  | 29 | 725 |

### III Semester-Organic chemistry

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Seminar

Total | 38  | 29 | 725 |

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Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
### III Semester-Physical chemistry

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### IV Semester-Inorganic chemistry

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Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
### IV Semester - Organic Chemistry

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I SEMESTER
PAPER-I: INORGANIC CHEMISTRY (1CHT1)
(Marks-100, Total hrs: 60)

**Unit I  Bonding theories of metal complexes:**
Crystal field theory: Salient features, splitting of d-orbitals in regular octahedral, distorted octahedral, square planar, tetrahedral, square pyramidal and trigonal bipyramidal geometries, Crystal field splitting energy, Pairing energy, High spin and low spin octahedral complexes, Calculation of crystal field stabilization energy (CFSE) in octahedral and tetrahedral complexes, Factors effecting the magnitude of crystal field splitting, Jahn-Teller distortion, general applications and limitations of crystal field theory, Special application of crystal field theory to spinels in site selection.

**Unit II  Reaction mechanisms of metal complexes:**
Energy profile of a reaction-Activated complex and Transition states, Inert and labile complexes, Lability and inertness of complexes in terms of Valence bond theory and Crystal field theory.
Types of substitution reaction mechanism - SN$_1$, SN$_2$, Id (Interchange dissociative) and Ia (Interchange associative).
Nucleophilic substitution reaction in octahedral complexes- Acid hydrolysis , factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Evidences in favour of conjugate base mechanism; Anation reactions.
Nucleophilic substitution reactions in square planar complexes- Mechanism of substitution, Trans effect, Theories of trans effect -Polarization theory and π–bonding theory, Applications of Trans effect in the synthesis of Pt(II) complexes.
Electron transfer reactions- Inner sphere and outer sphere mechanisms, Cross-reactions and Marcus-Hush theory.

**Unit III  Metal-ligand equilibria in solution:**
Solvation of metal ions, Metal complex formation in solution, Types of stability-concentration stability, conditional stability, thermodynamic stability and kinetic stability.
Step-wise stability constants and overall stability constant, Trends in stepwise stability constants. Factors influencing the stability of metal complexes with reference to metal
and the ligand, Chelate effect, and its thermodynamic origin, Macrocyclic effect of crown ethers and cryptates.

Hard and Soft acids and bases (HSAB) rule and its application to stability of complexes and metal-ligand interactions in the biological systems. Methods used for the determination of stability constants of metal complexes (Basic principles only) - Spectrophotometric, pH-metric and polarographic methods.

**Unit IV Magnetochemistry:**
Types of magnetism-paramagnetism, diamagnetism, ferromagnetism and antiferromagnetism, Temperature independent paramagnetism, Behaviour of para, dia, ferro and antiferromagnetic substances with temperature, Magnetic susceptibility measurement by Gouy method. Magnetic properties of metal ions- Origin of paramagnetic moment, spin moment and orbital moment, Quenching of orbital angular momentum by ligand fields; Orbital contribution to magnetic moment, Magnetic properties of metal complexes with A, E and T ground terms, Spin-orbit coupling contribution to magnetic moment, Spin cross-over in complexes.

Superconductivity: Introduction, magnetic properties of superconductors- Type I and Type II superconductors and Meissner effect. Applications of superconductors.

**Recommended books:**

Dean Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
1. a) Determination of total, permanent and temporary hardness of water  
b) Determination of COD of water  
c) Back titration of Ni\(^{2+}\) by EDTA  
d) Back titration of Al\(^{3+}\) by EDTA  
e) Substitution titration of Ca\(^{2+}\) by EDTA  
2. One component gravimetric estimations  
i) Estimation of Zn\(^{2+}\)  
ii) Estimation of Ba\(^{2+}\) (as BaSO\(_4\))  
3. Preparation of the following complexes and their characterization by metal estimation and conductance measurement  
i) \([\text{Cu(NH}_3\text{)}_4\text{SO}_4]\)  
ii) \([\text{Hg[Co(SCN)}_4]\)  
iii) \([\text{K}_3[\text{Fe(C}_2\text{O}_4)_3]\)  
iv) \([\text{Ni(en)}_3\text{S}_2\text{O}_3]\)  
v) \([\text{Co(NH}_3\text{)}_5\text{Cl}]\text{Cl}_2\)  
vi) \([\text{Mn(acac)}_3]\)  

**Scheme of valuation**

<table>
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<tr>
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<tr>
<td>Standardization</td>
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**Recommended Books:**  
1. Vogel's Text Book of quantitative chemical analysis (6\(^{th}\) edition)  
2. Analytical chemistry- Gary D. Christian (6\(^{th}\) edition)
Unit I  Stereochemistry-I:

Unit II  Reaction Mechanisms-I:

Unit III  Natural products-I:
**Unit IV  Heterocyclic compounds-I:**

Classification and nomenclature of the heterocycles based on the nature of the heteroatom and size of the ring. $\pi$-excessive and $\pi$-deficient heterocycles with suitable examples – comparative reactivity of furan, pyrrole, and thiophene (preparation not necessary). Synthesis, reactivity, and reactions of pyridine, chromone, coumarin, benzofuran, benzothiophene, indole, quinoline and isoquinoline.

**Recommended books:**

1. Stereochemistry of carbon compounds – E.L. Eliel
2. Stereochemistry of organic compounds – D. Nasipuri
3. Stereochemistry: conformation and mechanism – P.S. Kalsi
4. Reaction mechanisms – Jerry March
5. A guide book to reaction mechanisms in organic chemistry – Peter Sykes
11. Organic Chemistry – Paula Y. Bruice
12. Modern methods of organic synthesis – William Carruthers and Iain Coldham
15. Heterocycles – R.K. Bansal
16. An introduction to chemistry of heterocyclic compounds – R.M. Acheson
19. The higher terpenoids – Paul De Mayo
20. Mono- and sesquiterpenoids – Paul De Mayo
21. An introduction to chemistry of terpenoids and steroids – William Templeton
22. The alkaloids – Kenneth Walter Bentley
23. Alkaloids – S. William Pelletier
PAPER-VI: ORGANIC CHEMISTRY - PRACTICALS (1CHP2)
(6 Hours per week)

I. Some important techniques in practical organic chemistry: Recrystallization, mixed melting point, drying of solvents and steam distillation.

II. Preparation of
i) Methyl orange  
ii) Coumarin
iii) Pyrazolone  
iv) Azalactone

III. Preparation of
i) Benzanilide by Beckmann’s rearrangement:
   (a) Preparation of benzophenone oxime
   (b) Beckmann’s rearrangement to benzanilide
ii) Benzilic acid from benzoin:
   (a) Benzil from benzoin
   (b) Benzilic acid from benzil
iii) Anthranilic acid from phthalic anhydride:
   (a) Phthalimide from phthalic anhydride
   (b) Hoffmann’s rearrangement to anthranilic acid
iv) m-Nitroaniline from Nitrobenzene:
   (a) m-Dinitrobenzene from Nitrobenzene
   (b) m-Nitroaniline from m-Dinitrobenzene

Scheme of valuation
Marks: 75  
Time: 4Hrs

Single step preparation and Recrystallization  –  20
Two step preparation and Recrystallization  –  40
Viva, Record and Samples  –  15

Recommended books:
1) Vogel's textbook of practical organic chemistry – Arthur Israel Vogel, B. S. Furniss
2) Practical Organic Chemistry – Frederick George Mann and Bernard Charles Saunders
3) Advanced Practical Organic Chemistry – N K Vishnoi

Dean  
Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
I SEMESTER
PAPER-III: PHYSICAL CHEMISTRY (1CHT3)
(Marks-100, Total hrs: 60)

Unit I Thermodynamics – I:
Third law of thermodynamics, calculation of absolute entropies of solids, liquids, and gases – tests and exceptions. Standard entropies and entropy changes in chemical reactions, entropy of mixing, standard entropies of ions. Thermodynamic relations. Gibb’s and Helmholtz free energy, Standard free energy of formation. Variation of free energy with temperature and pressure. Free energy change in phase transformations – Clapeyron and Clausius-Clapeyron equation, Maxwell’s relationships and thermodynamic equation of state.


Unit II Electro Chemistry - I:


Unit III Kinetics – I:
Simultaneous reactions: Derivation of first order rate expression for parallel, opposing and consecutive reactions. Theory of absolute reaction rates – application to reactions

Dean Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
between atoms and molecules. Thermodynamic formulation of reaction rates–calculation of activation parameters.

Lindemann’s theory of unimolecular reactions and Hinshelwood modification–Effect of Solvent and Ionic strength on rates of ion-ion and ion-dipole reactions–Isotopic effect on reaction rates–substrate and solvent isotopic effect.

**Termolecular reactions**: Reactions of nitric oxide with hydrogen, oxygen, and halogens.


**Unit IV Quantum Chemistry–I**:
Planck’s quantum theory and derivation of Planck’s temperature radiation law–Derivation of time independent Schrödinger wave equation-wave function and significance of $\Psi$ and $\Psi^2$–Normalization and orthogonality of wave function – well behaved functions – Operators like linear momentum (p), angular momentum (L), Energy (E), Hamiltonian (H), operator $\nabla$ and $\nabla^2$. Properties of Hermitian operator. Eigenfunction, eigenvalue, commutation and eigen properties of angular momentum properties. Operator algebra – Postulates of quantum mechanics.

**Applications**: Application of Schrodinger wave equation to particle in a one-dimensional box and three-dimensional box, derivation of energy expressions – plots of $\Psi$ and $\Psi^2$– degenerate states – quantum mechanical tunnelling (qualitative treatment).

**Polynomials**: Hermite, Legendre, Associated Legendre, Laguerre and Associated Laguerre Polynomials (no derivation). Derivation of energy expression and wave function for a linear harmonic oscillator, plots of $\Psi$ and $\Psi^2$

**Recommended books**:  
1. Physical Chemistry by Donal D; Mcquarrie & John D Simon.  
2. Physical Chemistry by Peter Atkins and Julio de Paula  
3. Principles of Physical Chemistry by Samuel H.Maron and Carl F. Prutton  
4. Advanced Physical Chemistry by Gurdeep Raj  
5. Quantum Chemistry by R.K.Prasad  
6. Thermodynamics by Samuel Glasstone, D.Van  
7. Chemical Kinetics by K.J. Laidler  
9. An Introduction to Electrochemistry- Samuel Glasstone (10th Ed)  
10. Electrochemistry by M.S. Yadav  

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Dean
Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
Paper – VII  PHYSICAL CHEMISTRY PRACTICALS (1CHP3)  
(6 Hours per week)

1. **Kinetics:**
   (i) Acid catalyzed Acetone – Iodine reaction.  
   (Comparison of rate constants at different acid concentrations)
   (ii) Acid catalyzed hydrolysis of methyl acetate.  
   (Comparison of rate constants at different acid concentrations)
   (iii) Persulphate – Iodide reaction.  
   (Comparison of rate constants at different iodide concentrations)

2. **Polarimetry:**
   (i) Specific rotation of sucrose and glucose.
   (ii) Acid catalysed inversion of sucrose-Pseudo first order rate constants.  
   (Comparison of rate constants at different acid concentrations)

3. **Conductometry:** Titrations of
   a. (i) Strong acid and weak acid with Strong base.
   (ii) Mixture of strong and weak acids with Strong base.
   (iii) Strong acid and weak acid with Weak base.
   (iv) Salt with Strong base.
   b. Verification of Ostwald’s dilution law and determination of Ka.
   c. Solubility product of AgCl.

   b. Determination of molecular weights of polyethylene glycol or polyvinyl alcohol.

5. Determination of heat of solution of benzoic acid by solubility method.

**Scheme of valuation**

Marks: 75  
Time: 4Hrs

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<td>Principle record and viva</td>
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<td>15</td>
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</table>

**Recommended books:**
2. Practical Physical Chemistry by B. Vishwanathan and P.S. Raghavan,
3. Practical Physical Chemistry by B.D.Khosla and V.C. Garg.
4. Systematic Experimental Physical Chemistry -S.W. Raj Bhoj and Dr. T.K. Chondhekar

Dean

Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
I SEMESTER
PAPER-IV: APPLIED CHEMISTRY (1CHT4)
(Marks-100, Total hrs: 60)

Unit I  Reagents in organic synthesis:
Preparation and applications of the following reagents in organic synthesis and
functional group transformations: 1,3-Dithianes(Reactivity and umpolung effect),
Lithium disopropyl amide (LDA), Dicyclohexylcarbodiimide(DCC), Trimethylsilyl
iodide, Tri-n-butyl tin hydride, Dichloro dicyano benzoquinone (DDQ), Chloranil,
Selenium dioxide, Lindlar’s catalyst and Wilkinson’s catalyst Baker’s Yeast. Woodward-
Prevost hydroxylation, Phase transfer catalysts-Tetra alkyl ammonium halides, and
Crown ethers.

Unit II  Biomolecules:
Polypeptides and Proteins: Determination of structures of polypeptides – N-terminal
and C-terminal amino acid determination – Sequence determination in polypeptides –
polypeptide synthesis – Merrifield resins – Solid phase polypeptide synthesis.
Classification, structures, and functions of primary, secondary and tertiary proteins.
Carbohydrates: Determination of the relative and absolute configuration in D-glucose
and D-fructose. Structure elucidation and synthesis of Sucrose. Structural features of
Maltose, Lactose, Celllobiose, Starch, and Cellulose.

Unit III  Separation techniques:
Solvent Extraction Methods: General discussion, Liquid-liquid systems, Factors
favoring extraction of metal ions into organic solvents, quantitative treatment of solvent
extraction equilibria, synergistic extraction, Ion association complexes, Some practical
considerations in solvent extraction, Determination of Ni as Ni-DMG complex and of Pb
as Pb-dithizone complex; solid-liquid systems – Extraction of soluble solid compounds
by solvents.
Ion-Exchange Methods: General discussion, Typical synthetic Cation and Anion
exchange resins, Action of ion exchange resins, Ion exchange capacity, Determination of
cation and anion exchange resin capacities, Column operation and ion exchange
chromatography, Separation of Zn and Mg using anion exchange resin; Chelating ion
exchange resins, liquid ion exchangers.

Unit IV  Electro Analytical Techniques:
a)  Polarization and over-voltage, applications of over-voltage, over-potentials exchange
current density, derivation of Butler –Volmer equation, Tafel plot.
b)  Polarography: Dropping mercury electrode- Instrumentation - polarogram. Types of
Currents: Residual, Migration, and Limiting - Likovie equation. Types of limiting

c) Amperometric titrations: Principle and instrumentation. Types and application of amperometric titrations. Determination of $\text{SO}_4^{2-}$, metal ions viz., $\text{Mg}^{2+}$, $\text{Zn}^{2+}$, $\text{Cu}^{2+}$ and other substances.

d) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms-applications. Cyclic voltammetric study of insecticides (ex. Parathion)

e) Optical measurements: Refractometers, polarimeters, and colorimeters: Basic principles, instrumentation, and qualitative applications

**Recommended books:**

1. Reaction mechanisms – Jerry March
6. Carbohydrate chemistry – Davidson
7. Reagents for organic synthesis – Louis Fieser and Mary Fieser
8. Reactions Rearrangements And Reagents – S.N. Sanyal
9. Essential reagents for organic synthesis – Philip L. Fuchs, Andre B. Charette, Tomislav Rovis and Jeffrey W. Bode
10. Modern textbook of organic chemistry – Furguson
12. Principles of polarography- Kapoor
13. Principles of polarography- Heyrovsky
14. Modern electroanalytical methods – C. Charlot
15. Principles of physical chemistry – Gurudeepraj
20. Automatic methods of analysis, M. Valcarcel, M. D. Luque de Castro,
21. Principles of Instrumental Analysis, Skoog, Holler and Wieman,
II SEMESTER
PAPER-I: INORGANIC CHEMISTRY (2CHT5)
(Marks-100, Total hrs: 60)

Unit I  Electronic-spectra of metal complexes:
Free-ion terms and energy levels – Electron configuration, Microstates and Terms.
Calculation of microstates for \( p \) and \( d \) configurations, Russel-Saunders (L-S) coupling.
Derivation of terms for \( p^2 \) and \( d^2 \) configurations, Ground state term symbols for \( d \)
configurations, Hole formalism, Hund’s rules to determine ordering of energy levels,
Effect of weak fields on free ion terms, Selection rules governing electron transitions and
breakdown of selection rules, Orgel diagrams for \( d^1 \) to \( d^9 \) systems, Electronic spectra of
[\text{NiCl}_4]^{2-}\) complexes, Charge transfer Spectra, Calculation of ligand field parameters – Racah
parameter (\( B \)), Crystal field splitting (10DQ) and Nephelauxetic ratio (\( \beta \)).

Unit II  Organometallic Compounds:
Classification and nomenclature of organometallic compounds, Principles of synthesis of
organometallic compounds. Synthesis, structure and properties of organometallic
compounds of \( \text{Al} \) and \( \text{Sn} \). 18-electron rule and stability of organotransition metal
compounds. Synthesis, structure and bonding of olefin, allyl and cyclopentadienyl
organometallic compounds of \( \text{Fe}, \text{Pd} \) and \( \text{Pt} \). Applications of organometallic compounds
of \( \text{B} \) and \( \text{Si} \) in organic synthesis. Organometallic compounds in homogeneous catalysis
– Hydrogenation, Hydroformylation and Isomerization processes.

Unit III  Bioinorganic Chemistry:
Metal ions in biological systems – Brief survey of metal ions in biological systems,
Basic principles underlying biological selection of elements, Physiological effects of
metal ion concentration.
Oxygen transport and storage – Haemoglobin and Myoglobin, Geometric, electronic
and magnetic aspects of dioxygen binding, oxygen adsorption isotherms and
cooperativity, Physiological significance of hemoglobin, Role of globin chain in
haemoglobin.
Metals/ Metal compounds in medicine – Introduction, Metal deficiency and disease,
Iron deficiency, Zinc deficiency, and Copper deficiency; Metals used for diagnosis and
radiodiagnosis; Lithium, Gold and Platinum compounds used in therapy.
Unit IV  Ligational aspects of diatomic molecules:

Metal Carbonyls: Classification of metal carbonyls, General methods of preparing metal carbonyls, Ligational properties of Carbon monoxide (CO), Donor and acceptor molecular orbitals of CO, Bonding modes of CO, Evidence for multiple bonding, Eighteen electron rule, Electron counting methods i) Neutral atom method and ii) Oxidation state method, Structural and bonding aspects of Ni(CO)₄, Mn₂(CO)₁₀ and Fe₂(CO)₉.

Metal carbonyl clusters- Factors favouring metal-metal bond, Classification of metal carbonyl clusters, Structures of Fe₂(CO)₉, Co₂(CO)₈, Fe₃(CO)₁₂, Ru₃(CO)₁₂, Co₄(CO)₁₂, and Rh₆(CO)₁₆.

Metal nitrosyls: General methods of preparing metal nitrosyls, Donor and acceptor molecular orbitals of nitric oxide (NO), Bonding modes of NO, structural and bonding aspects of [IrCl(PPh₃)₂(CO)(NO)]⁺ and [RuCl(PPh₃)₂(NO)₂]⁺.

Metal dinitrogen complexes – Dinitrogen molecule (N₂) as a ligand, Molecular orbitals of N₂, Bonding modes - Terminal and Bridging, Structures of Ru (II) and Os (II) dinitrogen complexes.

Recommended books:

2. Introduction to ligand fields, B. N. Figgis, Wiley.
Paper – V INORGANIC CHEMISTRY PRACTICALS (2CHP4)

I. Estimations:
1. Glucose by using Fehling’s solution
2. Vitamin – C
3. Calcium in Milk
4. Iodine value of Oil
5. Chlorine in Bleaching Powder

II. Analysis of Binary Mixtures:
1. Determination of Cu$^{2+}$ and Ni$^{2+}$
2. Determination of Fe$^{3+}$ and Al$^{3+}$
3. Determination of Cu$^{2+}$ and Zn$^{2+}$
4. Determination of Ca$^{2+}$ and Mg$^{2+}$
5. Determination of Ferrocyanide & Ferricyanide

**Scheme of valuation**

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<td>Standardization</td>
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<td>Estimation of sample</td>
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<td>Viva, Record and samples</td>
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**Recommended Books:**
1. A Text Book of quantitative inorganic analysis (3rd and 6th editions)
II SEMESTER
PAPER-II: ORGANIC CHEMISTRY (2CHT6)
(Marks-100, Total hrs: 60)

Unit I  Named reactions in organic synthesis:
Beckmann rearrangement, Mannich reaction, Michael addition, Dienone-Phenol rearrangement, Robison annulation, Favorski reaction, Baylis-Hillman reaction, Shapiro reaction, Ugi reaction, Grubbs reaction, Heck reaction, Suzuki coupling, Stille coupling, Sonogashira coupling, and Buchwald reaction.

Unit II  Stereochemistry II:
Conformational analyses of Cycloalkanes: Conformations of small and medium sized rings and conformations of mono and disubstituted cyclohexanes. Factors governing the reactivity of equatorial and axial substituents attached to the cyclohexane ring – Relative stability and reactivity of conformational diastereomers – Stereochemistry of bicyclic systems involving five and six numbered rings. Conformations of cyclohexanone – Stereochemistry of addition to the carbonyl group in rigid cyclohexanone system.
Use of physical methods (dipole moment, IR and NMR) in determining the preferred conformers of simple organic molecules such as 1,2-dihalo ethanes, halohydrins and vicinal diols.
ORD studies: Optical rotation and optical rotatory dispersion, axial haloketone rule, octant rule, applications of ORD studies in the determination of configuration and conformation of organic molecules.

Unit III  Protection of functional groups and Nucleic acids:
Protection of functional groups: Principles of (1) protection of alcohols – Ether formation: methyl, benzyl, allyl, methoxy ethoxy methyl (MEM), THP, silyl, and TBDMS ethers; Ester formation– methyl, benzoyl, tosyl, and p-nitro benzoyl ester (2) protection of diols – acetal, ketal and carbamate formation (3) protection of carboxylic acids – Ester formation: methyl, benzyl, t-butyl, p-nitrobenzyl, p-bromophenacyl, and silyl esters (4) protection of amines – Amide and Carbamate formation with formyl, acetylation, benzoil, benzyloxy carbonyl (CBZ), tert-butylxycarbonyl (BOC), tert-butyl azido formyl, phthaloyl, di-tert-butyl pyrocarbonyl, Fluorenlymethyloxyxcarbonyl (FMOC), and triphenyl methyl groups (5) protection of carbonyl groups – acetal, ketal, 1,3-dioxolane, 1,3-dioxane, 1,3-dithiolane, 1,3-oxathiolane and 1,3-dithiane formation.
Nucleic acids: Isolations, structure, and properties of RNA & DNA – synthesis of nucleosides, nucleotides, and synthesis of polynucleotides. Biosynthesis of RNA and DNA.

Dean  Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
Unit IV Nonbenzenoid aromatic compounds:
Concept of aromaticity, Robinson’s sextet theory, Huckel’s rule, basis for the Huckel’s rule, limitations of the Huckel’s rule- Alternant and Non-alternant hydrocarbons Craig’s rule – Various Nonbenzenoid aromatic molecules – Synthesis and properties of aromatic 3,4,5,6,7,8-membered rings, metallocenes, annulenes, heteroannulenes, azulenes, fullerenes(C_{60}), Sydnones – Antiaromatic compounds,

Recommended Books:
1. Reaction mechanisms – Jerry March
3. Carbohydrate chemistry – Davidson
4. Textbook of organic chemistry – Morrison and Boyd
5. Organic reagents – Fieser and Fieser
6. Modern textbook of organic chemistry – Furguson
Identification of Organic compounds – Systematic qualitative analysis:
Physical data – Boiling points/ Melting points; Ignition test, Solubility classification, Detection of extra elements N,S and Halogens (Lassaigne sodium fusion test, Beilstein test). Functional group tests and preparation of two rational derivatives: Determine the melting points of solid derivatives and reference to literature to identify the compounds. A minimum of eight following compounds to be studied as unknown covering at least one from each of the solubility classes.

List of suggested compounds:
Glucose, Fructose, Benzaldehyde, p-Anisaldehyde, p-Chlorobenzaldehyde, Acetophenone, p-Nitroacetophenone, Benzophenone, Benzoic acid, p-Nitrobenzoic acid, p-Chlorobenzoic acid, Anisic acid, Phenol, p-Cresol, β-Naphthol, p-Chlorophenol, Aniline, p-Toluidine, p-Anisidine, o-Chloroaniline, m-Chloroaniline, Diphenylamine, N-methyl aniline N,N-dimethyl aniline, Benzamide, Ethyl benzoate, methyl benzoate, Nitrobenzene, Chlorobenzene, Bromobenzene, Naphthalene and Anthracene, Biphenylanthracene.

Scheme of valuation

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<td>Functional group test</td>
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<td>Preparation of derivatives</td>
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</tbody>
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Recommended books:
1. Vogel's textbook of practical organic chemistry – Arthur Israel Vogel, B. S. Furniss
2. Practical Organic Chemistry – Frederick George Mann and Bernard Charles Saunders
II SEMESTER
PAPER-III: PHYSICAL CHEMISTRY (2CHT7)
(Marks-100, Total hrs: 60)

Unit I Thermodynamics – II:
Statistical Thermodynamics: Thermodynamic probability of distinguishable and indistinguishable particles-most probable distribution—entropy and probability (Boltzmann–Planck equation), Maxwell–Boltzmann distribution law—partition function and types. Translational, rotational, vibrational and electronic functions—Relation between thermodynamic functions (E, H, S and G) and partition functions-factorization into translational, rotational, vibrational and electronic contributions of monoatomic and diatomic molecules. Sackur-tetrode equation of entropy. Equilibrium constant.

Unit II Solid State:
Defects in crystals: Point defects, colour centers, line defects and plane defects.
Specific heats of solids: Dulong and Pettit's law, Einstein theory and Debye theory of specific heats. Solid state reactions: Classification and theory of solid state reactions Δ-Wagner’s theory—examples.

Unit III Chemical Kinetics - II:
Effect of substituent on the rate of reaction—Hammett’s and Taft’s equations—use of σ and ρ constants and extended Hammett equation. Yukawa–Tsuno equation—Nonlinear Hammett’s Plots–Isokinetic temperature and its determination.
Acid-base catalysis: Homogeneous acid–base catalysis—mechanism of acid-base catalysis-protopylcic and prototropic mechanism.
Chain reactions: General Characteristics—Kinetics of Chain reactions—Mechanisms of thermal reaction of hydrogen with chlorine and bromine and their rate expressions—thermal decomposition of N₂O₅ and C₂H₆—general kinetic schemes—Inhibition of chain reactions by NO.
Unit IV  Quantum Chemistry - II:

Rigid rotator: Application of Schrodinger equation to rigid rotator— derivation of energy expression and wave function of a rigid rotator—solution of ($\phi$) and ($\theta$) parts of wave functions—total wave function of rigid rotator.

Hydrogen atom: Separation of (r), ($\phi$) and ($\theta$) equations—Solution of radial equation—Total wave function for hydrogen atom—radial and angular plots—probability functions and radial probability density plots for 1s and 2s orbitals.

Approximation methods: Variation method—principle and its application to hydrogen atom—perturbation method—First order correction terms of energy and wave function—application to particle in a one-dimensional box under an electric field.

Bonding in molecules: Born-oppenheimer approximation – construction of molecular orbitals by LCAO. MO theory of H$_2^+$ ion. Energy and wave function expressions (no derivation). Basic postulates of Huckel’s $\pi$ electron theory and its applications to ethylene system.

Recommended books:

1. Physical Chemistry by Donal D; Mcquarrie & John D Simon.
2. Atomic Structure and the Chemical Bond including Molecular Spectroscopy –Manas Chanda (4th edn)
3. Physical Chemistry - Peter Atkins and de Pulpa Oxford University Press.
6. Quantum Chemistry - R.K.Prasad
7. Thermodynamics - Samuel Glasstone
8. Chemical Kinetics by K.J. Laidler
1. **Potentiometry:**
   a. **Acid–base titrations:**
      (i) Strong acid with strong base.
      (ii) Weak acid with strong base and determination of $pK_a$ of weak acid.
      (iii) Mixture of acids with strong base.
   b. **Redox titrations:**
      (i) Ferrous ion with KMnO$_4$ or K$_2$Cr$_2$O$_7$
      (ii) Ferrous ion with Ce$^{4+}$
   c. **Precipitation titrations:**
      (i) KCl or KI with AgNO$_3$
      (ii) Mixture of (KCl + KI) with AgNO$_3$

2. **Colorimetry:**
   Verification of Lambert-Beer’s law and determination of molar extinction coefficient of KMnO$_4$, CuSO$_4$, K$_2$Cr$_2$O$_7$, Cu (NH$_4$)$_6$SO$_4$
   3. Verification of Freundlich adsorption isotherm-Acetic acid–activated charcoal system
   4. Distribution of Iodine between CCl$_4$ and aqueous KI. (determination of unknown concentration of KI)
   5. Determination of partial molar volume of methanol in aqueous methanol.

**Scheme of valuation**

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**Recommended Books:**

2. Practical Physical Chemistry - B. Vishwanathan and P.S. Raghavan,

Dean's signature
Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
II SEMESTER
Paper-IV: Spectroscopy (2CHT8)
(Marks-100, Total hrs 60)

Unit I  Symmetry & Group Theory:
Introduction- concepts of symmetry in molecules, symmetry elements, symmetry operations, mathematic rules of a group – abelian and non-abelian groups. Point groups-classifications of point groups- Exercises on molecular point groups -H₂O, o-C₆H₄X₂, C₂H₅N, CH₃Cl, H₂O₂, CH₄, B(OH)₃, C₂H₂Cl₂[PtCl₄]²⁻, C₃H₄(Allene), [FeCl₆]³⁻, Metallocenes (Eclipsed and Staggered). Descent in symmetry of molecules with substitution (H₂O, HOD, CH₄, CH₃X). Symmetry criteria of optical activity, Symmetry restrictions of dipole moment, group multiplication table – subgroups.

Unit II Microwave & Electronic Spectroscopy:


Unit III Infrared and Raman Spectroscopy:

**Raman spectroscopy:** Raman effect-Quantum theory-selection rules-Rotational and Vibrational Raman effect. Instrumentation, Mutual exclusion principle and Raman spectra of $\text{Hg}_2^{2+}$, $\text{NO}_3^-$, $\text{ClO}_3^-$, $\text{N}_2\text{O}$, $\text{CO}_2$ and $\text{CH}_4$.

**Unit IV  NMR Spectroscopy and ESR Spectroscopy:**


**Electron spin resonance spectroscopy (ESR):** Introduction-Principles involved in ESR spectroscopy. Instrumentation, presentation of ESR spectra, hyperfine coupling constant. ESR spectrum of hydrogen atom. Lande’s splitting factor and its significance. ESR spectra of organic radicals like methyl, ethyl, isopropyl, benzene (anion and cation radicals), 1,4-benzoquinone and naphthalene anion.

**Recommended Books:**

5. Spectroscopy organic compounds-P. S. Kalsi (New Age International).
6. Organic Spectroscopy-Jag Mohan (Narosa)
15. Applications of spectroscopy-J. Dyer.
III Semester
Paper-I SPECTROSCOPY (3CHT9)
(Common paper for all specializations)
(Marks 100, Total Hours 60)

Unit-I NMR spectroscopy:
Applications of spin-spin coupling in determination of structure and stereochemistry of organic molecules, NOE and its applications, and Lanthanide shift reagents. Recording of $^{13}$C NMR spectra (PFT technique), Types of $^{13}$C NMR spectra: Undecoupled, proton decoupled, selective proton decoupled spectra and off-resonance decoupled spectra – Spin decoupling method-Double resonance. $^{13}$C chemical shifts and factors affecting the chemical shifts. Calculation of chemical shifts of alkanes, alkenes and alkynes. Applications of $^{13}$C NMR spectra in structure determination of organic molecules. Editing techniques: INEPT and DEPT methods.

2D NMR techniques: Principles of 2D NMR, Different types of 2D-experiments with suitable examples. Correlation spectroscopy (COSY): HOMOCOSY ($^1$H-$^1$H COSY) and HETERO- COSY ($^1$H-$^{13}$C COSY), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D– INADEQUATE experiments.

Unit-II Mass Spectroscopy:
Origin of mass spectrum, principles of EI mass spectrometer- Instrumentation. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, metastable ion peaks, determination of molecular formula and High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds – $\alpha$-cleavage, $\beta$-cleavage, McLafferty rearrangement, Retro-Diels-Alder fragmentation and ortho effect. Fragmentation pattern of individual heterocyclic systems viz., Furan, Pyrrole, Thiophene and Pyridine. Preliminary account of chemical ionization.

Unit-III Photoelectron, AUGER Electron & Mössbauer spectroscopy
A) Photoelectron spectroscopy – Principles, Koopman’s theorem, Block diagram of photoelectron spectrometer. Ultraviolet photoelectron spectroscopy (UPS), Applications of UPS to $\text{O}_2$ and $\text{N}_2$ molecules. X-ray photoelectron spectroscopy (XPES/ESCA), Chemical shift, Applications of XPES in qualitative analysis, Structural analysis and surface studies.

B) AUGER electron spectroscopy – Principles, Instrumentation and Applications
C) Mössbauer Spectroscopy–Principles, Block diagram for experimental set-up. Recording Mössbauer spectrum, Isomer shift, Quadrupole interactions and Magnetic interactions, Applications of Mössbauer spectroscopy in the study of iron and tin compounds.

**Unit-IV** Combined application of UV, IR, $^1$H-NMR, $^{13}$C -NMR and Mass spectra:
Introduction to the analytical approach towards the structure elucidation of simple organic molecules by combined application of UV, IR, $^1$H-NMR $^{13}$C-NMR and Mass spectra.

**Recommended Books:**
1. Instrumental methods of Analysis– Willard, Dean & Settle.
2. Principles of Instrumental Analysis – Skoog, Holler and Wieman
3. Introduction to photoelectron spectroscopy – P. K. Ghosh
4. Applications of Mössbauer Spectroscopy – Green Wood
5. Structural inorganic chemistry-Mössbauer spectroscopy – Bhide
6. Spectroscopic identification of organic compounds– Silverstein, Basseler and Morril
8. NMR in chemistry -A multinuclear introduction – William Kemp
10. Spectroscopic methods in Organic chemistry – DH Williams and I Fleming
11. Modern NMR techniques for chemistry research – Andrew B Derome
12. Introduction to organic spectroscopy – Pavia
14. Nuclear Magnetic Resonance Basic principles – Atta-Ur-Rahman
17. Physical methods for chemists– R.S. Drago, 2nd ed. (Saunders College Publishers)
18. Spectroscopy of organic compounds- P. S. Kalsi

Dean Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
III Semester
Paper-II Synthetic Organic Chemistry-I (3CHT10)
(Common paper for all specializations)
(Marks 100, Total Hours 60)

Unit-I Organic Photo Chemistry:
Photo excitation of molecules-Electronic transitions and types of electronic transitions, Energies and life times of excited states, Fate of excited molecules, Photophysical processes-Jablonski diagram. Photochemical sensitization and Photochemical quenching.

Photochemistry of carbonyl compounds— Photoreductions (Intermolecular and Intramolecular), Paterno-Buchi reaction (Intermolecular and Intramolecular including stereochemistry) and limitations. Photochemical cleavages–Norrish Type-I and Norrish Type-II reaction (including stereochemistry). Photochemistry of Olefines–Cis-Trans isomerisation, Dimerisation, Simple additions and, Inter and Intra molecular cyclo additions. Electrocyclisation and Cycloaddition reactions in conjugated dienes. Photochemistry of Aromatic compounds—Ring isomerisation, Photocyclo additions. Photorearrangements-Barton reaction, Zimmermann rearrangement, Photo-Fries rearrangement, and Migration of groups in aromatic compounds.

Unit-II Pericyclic Reactions:
Introduction –Characteristics and classification of pericyclic reactions. Representation of molecular orbitals-Bonding, Non bonding and Anti bonding, Symmetry properties with special reference to plane of symmetry and two fold axis of symmetry. FMO, Orbital Correlation Diagram(OCD) approaches and Stereochemistry of Electrocyclic reactions (4n and 4n+2 electron system), Cyclo addition reactions (4n & 4n+2 systems and including 1,3 Dipolar cycloaddition in ketenes). Detail study of Diels-Alder reaction –Stereochemistry –Cis-rule – Alder’s Endo rule and Regioselectivity. Elementary treatment of PMO approach. PMO, FMO approach and Stereochemistry of Sigmatropic rearrangements-[1,3], [1,5], [1,7], Cope, Oxy-Cope, Aza-Cope, Claisen, and Aza-Claisen rearrangements. Sommlet-Hauser reaction, Chelotropic reactions (Additions and Eliminations), Group transfer, Group elimination and Ene reactions. Exercises based on pericyclic reactions.

Dean
Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
**Unit-III Formation of \(-C-C-\) and \(-C=C-\) bonds:**

C-C (single) bond formation: Alkylation of relatively acidic methylene group-Enolate anions- Alkylation of enolate anions and Stereochemistry of alkylation of enolate anions – Aldol addition reactions of Li, B, Ti enolate anions and Mukaiyama reaction. Conjugate addition of Grignard reagents in presence of copper salts. Synthetic applications of Gilman reagent in C-C bond formation -Reaction with halides, sulfonates, epoxides and \(\alpha,\beta\)-unsaturated carbonyl compounds, esters and epoxides. The enamine reactions in C-C bond formation–Synthetic applications of carbenes and carbenoids.


**Unit-IV Oxidation and Reductions:**

**Oxidations:** Oxidation of C=C with transition metal oxidants – KMnO4 and OsO4, Epoxidation with peroxy acids, and hydroperoxides and subsequent transformation of epoxides. Stereochemistry of perhydroxylation(cis and trans) – Cleavage of glycols [HIO4 and \(\text{Pb(OAc)}_4\)]. Oxidation of alcohols to carbonyl compounds using \(\text{Cr}^{\text{VI}}\) oxidants-(PCC, PDC, Collins reagent, and Jones reagent) and Swern oxidation. Singlet oxidation– Generation of Singlet oxygen- Reaction of alkenes with Singlet oxygen and their subsequent transformation. Synthetic applications of hypervalent Iodine: 2-Iodoxybenzoic acid (IBX), Dess-Martin oxidation, and Iodobenzenediacetate.

**Reductions:** Group III-hydride transfer reagents: NaBH4, NaBH3CN, LiAlH4, Lithiumhydrido alkoxyaluminates and DIBAL to reduce carbonyl groups and other functional groups– Reduction of \(\alpha,\beta\)--unsaturated ketones(1,2 and 1,4-additions) Stereochemistry of hydride reductions (Cyclohexanones).

Group IV hydride donors: Trialkylsilanes (\(\text{R}_3\text{SiH}\) and \(\text{Ar}_3\text{SiH}\)) to reduce hindered alcohols and carbonyl compounds, HCOOH -Eschweiler–Clarke reaction and Hydride ion transfer in MPV reduction and Cannizzaro reaction.

Dissolving metal reductions: a) Addition of hydrogen–Metal in liquid NH3 and alcohol – reduction of carbonyl functional group and \(\alpha,\beta\)--unsaturated ketones, partial reduction of aromatic rings and Birch reduction.

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b) Reductive removal of functional groups-reductive removal of halogen, carbonyl group, acetate and sulfonate groups with Li or Na/EtOH, Diethyl phosphorochloridate, Zn-Hg/HCl, Zn-Al/AC₂O and Zn-Al/NH₄Cl.

c) Reductive C-C and C=C bond formation—Formation of diols, cyclic diols, alkenes, cycloalkenes by reduction of carbonyl group with Mg-Hg, Mg-Hg/TiCl₄, Na/TiCl₄, and Zn or Cu/TiCl₄. Reductive coupling of esters with Na/Me₃SiCl in Xylene and Acyloin condensation- construction of small and large ring size cycloalkanes by reduction of diesters.

**Recommended Books:**

1. Molecular reactions and photochemistry – C. Dupey & O. L. Chapman
2. Molecular photochemistry – Turro
3. Molecular Photochemistry – Gilbert & Baggo
4. Organic Photochemistry – D Coyle
5. Molecular Reactions and Photochemistry – Depuyand Chapman
6. Photochemistry – C W J Wells
7. Some modern methods of organic synthesis – W. Carruthers
10. Organic synthesis – M. B. Smith
12. March's Advanced Organic Chemistry – Michael B. Smith
13. Conservation of Orbital Symmetry – Woodward and Hoffmann
14. Organic Reactions and Orbital Symmetry, – Gilchrist and Storr
15. Pericyclic Reactions — a problem solving approach— Lehr and Merchand
17. Pericyclic Reactions – Mukherjee S M
Unit-I Metalloproteins and Metalloenzymes:
General principles in metal binding sites – preservation of electroneutrality, self-
assembly of metal clusters. Metalloproteins–Electron transfer proteins: Ferridoxins,
Rubredoxins, Blue copper proteins, Cytochrome C. Metalloenzymes –
Carboxypeptidase A, Carbonic anhydrase, Vitamin B_{12}, Cytochrome P450.

Unit-II Metal ion transport and storage:
Transport of iron by transferring, storage of iron by Ferritin, synthetic iron-oxo
aggregates, Transport of iron by siderophores (Hydroxymate and phenolate
siderophores), Models for siderophores; Transport of copper by ceruplasmin and serum
albumin; transport of Na and K ions across cell membranes by Na\(^+\) - K\(^+\) ATPase;
Transport of Ca across sarcoplasmic Reticulum by Ca\(^{2+}\) - AT Pase; storage and transport
of Vanadium.

Unit-III Metal complexes and their interaction with nucleic acids:
Structure of nucleic acids, Interaction of metal complexes with nucleic acids –
Coordination, Intercalation and Hydrogen bonding; Fundamental reactions with
nucleic acids – Redox chemistry and Hydrolytic chemistry; Nuclease activity of tris
(Phenanthroline) metal complexes and their interaction with DNA; Applications of
nuclease activity of metal complexes as spectroscopic probes, metallo printing reagents,
conformational probes and cleavage probes; Metal-nucleic acid interactions in nature-
Structural role, Regulatory role and Pharmaceutical role.

Unit-IV Supramolecular Chemistry:
Concepts and principles, Host-Guest Chemistry, Non-covalent bonds, crown ethers,
cryptands and their metal complexes, Molecular recognition for different types of
molecules, spherical recognition, Tetrahedral recognition, cooperativity and
multivalency, Design and synthesis of co-receptor molecules and multiple recognition,
supramolecular reactivity and catalysis, supramolecular devices, supramolecular
photochemistry.
**Recommended Books:**

2) Inorganic biochemistry, Vols I & II Ed. - G.L. Eichorn.
5) Inorganic biochemistry - J.A. Cowan, VCH Publications.
6) Supramolecular Chemistry - J.M. Lehn.
III Semester - Inorganic Chemistry (Specialization)
Paper – IV Inorganic Photochemistry and Chemistry of Materials (3CHT 12)
(Marks 100, Total Hours 60)

Unit-I Inorganic Photochemistry:
Basics of photochemistry – Absorption of light and molecular excitation, photochemical laws and Quantum yield; Electronically excited states and their life-time measurements, properties of excited states – structure, Acid-base strength and Reactivity; Excited states of metal complexes, comparison with organic compounds, Electronically excited states of metal complexes, charge transfer states; photochemical reactions of metal complexes – photosubstitution (photoaquation and photoexchange), Photoionization, Photoisomerization; Photochemical decomposition of water using CdS and Ru-bipyridyl complex.

Unit-II Chemistry of Materials:
Ceramics – Introduction, structures, classification and Applications of ceramics
Dielectrics – Types and mechanism of polarization, Ferroelectrics, Hysteresis loop of ferroelectrics, Pyroelectrics, Piezoelectrics, Relation between ferroelectricity, pyroelectricity and piezoelectricity, Applications of ferro-, Pyro- and piezoelectrics.

Unit-III Nanomaterials – I:
Introduction to nanoparticles, Classification of nanoparticles, Preparation of nanoparticles – Bottom-up approach, To-down approach, chemical vapour deposition method, Thermolysis method, Pulsed laser method; Optical and electrical properties of nanomaterials, characterization of nanomaterials – X-ray spectroscopy, Scanning electron microscopy, Transmission electron microscopy, Atomic force microscopy, Field ion microscopy; properties and various applications of ZnO, iron and gold nanomaterials.

Unit-IV Nanomaterials – II:
Dendrimers–Introduction to dendrimers, synthesis, structure, properties and applications of dendrimers.

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Recommended Books:

1. Concepts of inorganic photochemistry- Adamson and Fleichner
2. Elements of inorganic photochemistry- Ferrandi.
6. Nanomaterials and nanochemistry - C.Brechigneae, P. Houdy and M. Lahmai (Eds.), Springer.
8. The most beautiful molecule – The discovery of the Buckyball, H.A. Williams, John Wiley & Sons, Inc.
III Semester – Inorganic Chemistry Practicals (Specialization)

Paper-V Preparation of Complexes and their characterization by Physiochemical techniques (3CHP7) (Marks 100, 9 Hours per week)

1. \([\text{Cu} (\text{NH}_3)_4\text{SO}_4\cdot\text{H}_2\text{O}]\)
2. \([\text{Ni(DMG)}_2]\)
3. \([\text{Mn(acac)}_2]\)
4. \(\text{Na[Cr(\text{NH}_3)_2(\text{SCN})_4]}\)
5. Prussian blue, Turnbull’s blue
6. \([\text{Co(NO}_2)(\text{NH}_3)_3]^{2+}\) and \([\text{Co(ONO)(NH}_3)_5]^{2+}\)

Paper-VI Analysis of Ternary mixtures and Complex materials (3CHP8)
(Marks 100, 9 Hours per week)

I. Analysis of Ternary mixtures
1. \(\text{Ag}^{+}, \text{Cu}^{2+}, \text{and Ni}^{2+}\)
2. \(\text{Cu}^{2+}, \text{Ni}^{2+}\) and \(\text{Zn}^{2+}\)
3. \(\text{Fe}^{3+}, \text{Mg}^{2+}, \text{and Ca}^{2+}\)

II. Analysis of Complex materials
1. Brass
2. Devarda’s alloy
3. Cement

Recommended Books:
2. Comprehensive experimental chemistry- V.K. Ahluwalia, New publication

Scheme of Valuation

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Dean Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
Unit-I Heterocyclic Chemistry-II:
Synthetic methods and reactivity of the following five membered heterocyclic systems: Carbazoles, Pyrazoles, Indazoles, Imidazoles, Benzimidazoles, Oxazoles, Benzoazoles, Isoxazoles, Thiazoles and Benzthiazoles.

Unit-II Reaction Mechanisms-III:
Study of the following special mechanistic aspects in organic chemistry

Unit-III Combinatorial synthesis:

Unit-IV Green Chemistry:
phase-transfer catalysts – Reactions without solvent, support or catalyst. Microwave activation-benefits and limitations. Examples of reactions on solid supports, reactions without support or catalyst.

**Recommended Books:**

1. Heterocyclic chemistry - R. K. Bansal
2. Heterocyclic Chemistry - T. Gilchrest
3. An introduction to the Chemistry of heterocyclic compounds - R.M. Acheson
4. Heterocyclic Chemistry - J.A. Joule & K. Mills
5. Principles of Modern Heterocyclic Chemistry - A. Paquette
7. Green chemistry, Theory and Practical - Paul T. Anastas and John C. Warner
10. Analytical Methods in Combinatorial Chemistry (Critical Reviews in Combinatorial Chemistry) - Bing Yan
15. March's Advanced Organic Chemistry – Michael B. Smith
Unit-I Classification, Isolation, Separation and Identification of Natural products:
Classification within each type of natural products (classification of alkaloids, classification of terpenoids, steroids, quinonoids, flavanoids...etc.) – General techniques of isolation and purification of natural products (with suitable examples representing different types of natural products) – Color reactions, spot tests and other basic identification techniques in natural products (with reference to flavanoids, terpenoids, alkaloids, quinine pigments, steroids etc.) – Basic separation techniques used in various types of natural products.

Unit-II Chemistry of Terpenenoids:
Structure elucidation and total synthesis of Farnesol, Zinziberene, Cadinene, Abietic acid, Lanosterol and β-Amyrin.

Unit-III Chemistry of Alkaloids:
Structure elucidation and total synthesis of Ephedrine, Cocaine, Narcotine, Morphine, Codeine, Thebaine, Reserpine and Strychnine.

Unit-IV Chemistry of Steroids:
Structure, stereochemistry and synthesis of Cholesterol, Androsterone, Testosterone, Oestrone, Oestradiol, Oestriol, Progesterone and Cortisone.

Recommended books:
1. Textbook of organic chemistry - I L Finar Vol II
2. An introduction to the chemistry of terpenoids and steroids - William Templeton
4. Steroids - Fieser arid Fieser
6. Alkaloids - Bentley
8. The chemistry of terpenes - A Pinder
9. Terpenoids - Mayo
11. Alkaloids - Pelletier
12. Total synthesis of Natural Products - Apsimon (Vol 1-5)
III Semester - Organic Chemistry practicals (Specialization)

Paper-V Preparation of organic compounds and Spectral analysis (3CHP9)
(Marks 100, 9 Hours per week)

(A) Two step preparation:
1. \(\text{o-chlorobenzoic acid}\) form \(\text{anthranilic acid}\)
2. \(\text{p-Bromoaniline}\) from acetanilide
3. \(\text{p-Nitroaniline}\) from acetanilide
4. \(\text{Tri bromobenzene}\) from \(\text{aniline}\): (a) \(\text{Aniline to tribromoaniline}\) (b) \(\text{tribromoaniline to tribromo benzene}\)
5. Preparation of 2,4-DNP: (a) Chlorobenzene to 2,4-dinitrochlorobenzene (b) Preparation of 2,4-DNP from 2,4-dinitrochlorobenzene
6. Preparation of Iosin: (a) Fluorosin from phthalic anhydride (b) Iosin from fluorosin.

(B) Spectroscopic identification of some organic compounds:
A set of spectral analytical data for at least 20 compounds will be analyzed by each student and two out of the same compounds will be chosen for the examination from which the student will analyze and identify one compound.

Scheme of Valuation
Marks 100 Time: 4Hours
Experiments (2) 80 Marks
Record/ Sample & Viva 20 Marks

Paper-VI: Organic mixture analysis (with two component mixture) (3CHP10)
(Marks 100, 9 Hours per week)

Organic mixture analysis (With two component mixture): Separation of the two component mixture of organic compounds in a systematic procedure and systematic identification of each of the component organic compounds by using: Preliminary examination, identification of extra elements, common functional group tests, specific functional group tests, preparation of at least two rational derivatives and finally identifying the given compounds by checking the melting points of its derivatives with those in literature.

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Mixture for analysis:
1) Strong Acid + Neutral
2) Base + Neutral
3) Weak acid + Neutral
4) Neutral + Neutral

At least ten mixtures have to be analyzed by the students.

**Recommended Books:**

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin
4. Practical organic chemistry by Mann & Saunders
5. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster

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<td>Separation of mixture</td>
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<td>*Tests for two components</td>
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*Note: For each component, identification of functional group, extra elements, determination of melting point and preparation of derivatives -30 marks
III Semester-Physical Chemistry (Specialization)
PAPER-III  Quantum Chemistry, Kinetics & Electrochemistry (3CHT15)
(Marks 100, Total Hours 60)

Unit-I  Quantum Chemistry – III:
MO diagrams and MO configurations of Homo nuclear diatomic molecules
H\textsubscript{2}, Li\textsubscript{2}, N\textsubscript{2}, O\textsubscript{2}, F\textsubscript{2} and heter diatomic molecules HF, BN, CO, NO.
LCAO treatment of H\textsubscript{2}\textsuperscript{+} and H\textsubscript{2} by VB theory and MO theory wave functions and energy expressions, Comparison of VBT and MOT of Bonding with reference to H\textsubscript{2} molecules.
Angular momentum- Ladder operators, addition of angular momenta spin, anti symmetry and pauli exclusion principle.

Unit-II  Quantum Chemistry – IV:
Concept of hybridization, quantum mechanical treatment of SP, SP\textsuperscript{2} and SP\textsuperscript{3} hybrid orbitals, Wave functions and angles. Hybrid orbitals on oxygen in H\textsubscript{2}O. HMO theory of conjugated polyenes. Application to allylsystems, butadiene, cyclopropenyl and cyclobutadiene systems energy and wave functions-Applications of HMO coefficients to calculate electron density, charge density, bond order. HMO theory of hetero aromatic compound of pyrrole.

Unit-III  Kinetics:

Unit-IV  Electro Chemistry:
Electro kinetic phenomenon, electrical double layers,(Helmholtz and stern potential),Zeta potential and its determination – Electro osmosis and streaming potential, electro capillary phenomena.
Ion selective electrodes- Membrane electrodes, theory of glass membrane potential.

**Recommended books:**

3. Quantum chemistry - D.A.Mcquarrie, Viva Books Pvt.,Ltd.,
5. Advanced physical chemistry by Gurudeep raj Goel Publishers House,Meerut.
9. Text book of physical chemistry -Puri& Sharma
10. Text book of advanced physical chemistry - Gurudeepraj
11. Electrochemistry,-S.Glasstone.
Unit-I  Group Theory:
Symmetry operations forming a group. Matrix representation of symmetry operations and point groups, isomorphism, Reducibleand irreducible representation. The great orthogonality theorem (without proof) and its properties for reducible and irreducible representation. Relation between reducible and irreducible representation.
Character tables – construction of character tables for C\(_2\)V and C\(_3\)V groups- Direct product rule, Group theoretical approach for UV transitions in ethylene and formaldehyde. IR and Raman active modes of water molecule.

Unit-II  Diffraction Studies:
Neutron diffraction: Scattering of neutrons, magnetic scattering, Elucidation of structure of magnetically ordered unit cell. Application and limitations.

Unit-III  Spectroscopy –I:
Photoelectron spectroscopy: Basic principles, photo-electric effect, ionization process, Koopmans theorem, PES of Simple molecules, XPES, Chemical shift applications and ESCA.
Photo acoustic spectroscopy: Basic Principles of PAS-PAS of gases and condensed systems chemical and surface applications.
Electron-Spin resonance spectroscopy: Zero-field splitting- kramer’s degeneracy – McConnell relationship, double resonance technique (ENDOR). ESR spectra of transition metal complexes
ORD and CD Spectroscopy: Basic concepts of optical rotatory dispersion (ORD) and circular dichroism (CD), Deduction of absolute configuration–Cotton effect–Octant rule for ketones. Applications of ORD and CD spectroscopy.

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Unit-IV Spectroscopy –II:
13C-NMR: General considerations 13C-NMR & 1H-NMR- Chemical shift (aliphatic, olefinic, alkyne, aromatic and carbonyl carbon). Coupling constant and factors affecting it. Splitting of 13C-NMR signals and simplication of signals by decoupling methods. Examples of 13C-NMR spectra.

ATR spectroscopy: Basic principle, total internal reflection instrumentation and applications.


Recommended books:
III Semester  Physical Chemistry-Practicals (Specialization)

Paper-V  –Kinetics (3CHP11)  
(Marks 100,  9 Hours per week)

1. Persulphate -Iodide reaction –Determination of
   a. Order  b. Solvent Effect  c. Salt effect  d. Temperature effect
   e. Catalytic effect using  Ferric in presence of Copper.

III Semester  Physical Chemistry-Practicals (Specialization)

Paper-VI  Instrumentation (3CHP12) (Marks 100, 9 Hours    per week)

I. Potentiometry / $\text{pH}$ Metry
   1. Titration involving dibasic and tribasic acids.
   2. Redox reactions and mixture of metal ions.
      a. $(V^{5+} + Mn^{7+})$ by $Fe^{2+}$
      b. $(V^{5+} + Ce^{4+})$ by $Fe^{2+}$
   3. Single Electrode potential
   4. Precipitation titration
      a. $KCl$ Vs $AgNO_3$  b. $(KCl +KI)$ Vs $AgNO_3$
      c. $(KCl +KBr + KI )$ Vs $AgNO_3$
   5. Isoelectric point of Glycine.
   6. Verification of Gibbs- Helmohltz equation.
   7. $P^{Ka}$ of Chloro acetic acid.

II. Colorimetry:
   1. Estimation of $Cu^{2+}$ by EDTA (Mono and bivariation methods)
   2. Estimation of $Ni^{2+}$ by EDTA (Mono and bivariation methods)
   3. Estimation of $Fe^{2+}$ by complexing with (1,10 phenanthrolin)
   4. Determination of $Cu^{2+}$ and $Fe^{3+}$ in the given mixture by EDTA
Recommended books:
1. Practical physical chemistry by A. Findlay, Longman-London
2. Practical physical chemistry by B. Vishwanthan and P.S. Raghavan.
3. Practical physical chemistry by B.D. Khosla and V.C. Gard, R.Chand or Co.Delhi.

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Dean
Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
III Semester
Environmental Chemistry (Open elective) (3CHO1)
(Marks-100, Total hrs: 60)

**Unit-I Environment and Natural cycles:**

**Unit-II Air pollution and its control measures:**
Air pollution and sources of air pollution, Air pollutants, Chemical and photo chemical reactions in the atmosphere, Acid rain, Green house effect; Major sources of green house gases, Emission of carbon dioxide, Correlation of rise in temperature with increasing atmospheric carbon dioxide concentration, Impact of green house effect on global climate, Other consequences of green house effect, Control and remedial measures of green house effect; Ozone depletion, Causes and consequences of ozone depletion, Mechanism of ozone depletion by chemicals, Control and remedial measures of ozone depletion; Photochemical smog.

**Unit-III Water pollution and its control measures:**
Water quality parameters: Dissolved oxygen demand and Chemical oxygen demand; water pollution, Signs of water pollution, water pollutants; Sources of water pollution: Domestic wastes and their harmful effects, Industrial wastes and their harmful effects; Sewage treatment: Domestic sewage treatment, Industrial sewage treatment; Treatment of drinking water: Sedimentation, Coagulation, Filtration, Disinfection, Removal of colour and odour, Destruction of algal and fungal growth, Deflouridation by adsorption process.

**Unit-IV Soil pollution and Radio active pollution and their control:**
Soil pollution and Soil pollutants, Adverse effects of soil pollution, Mining and soil pollution, Sources and adverse effects of solid waste. Solid waste disposal methods: Open dumping, Ocean dumping, Land filling, Recycling and Composting.

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Radioactive Pollution: Sources of radioactive pollution, Adverse effects of radioactive pollution, Control measures of radioactive pollution, Disposal methods of radioactive wastes.

**Recommended books:**

1. Environmental chemistry, A.K.De
2. Environmental chemistry, B.K. Sharma and H. Kaur
3. Environmental chemistry, J.W. Moore and E.A. Moore
M.Sc Chemistry-IV Semester

Paper – I Analytical and Physical Chemistry (4CHT17)
(Common paper for all specializations) (Marks 100, Total Hours 60)

Unit-I Chromatography:

Chromatographic methods: Geneal discussion, Adsorption and partition chromatography, component identification parameters, Theories of Chromatographic separations – Plate theory and Rate theory; chromatographic process optimization, Retention analysis, Resolution, principles and applications of paper chromatography and thin layer chromatography, Gas-Liquid chromatography, High performance liquid chromatography and supercritical fluid chromatography – Principles, instrumentation, detectors used and applications; Hyphenated techniques – Gas chromatography – Mass spectrometry and liquid chromatography – Mass spectrometry, principles and applications.

Unit-II Thermoanalytical methods:

Introduction to thermoanalytical methods, Thermogravimetric analysis (TGA), Principles, Derivative thermogravimetry (DTG), Comparison and interpretation of TG and DTG curves, Instrumentation of TG, TGA curves of individual compounds and mixtures, Factors affecting TGA curves, Applications of TGA. Differential thermal analysis (DTA) – Principles, Instrumentation, Interpretation of DTA curves, Influence of atmosphere on DTA curves of a sample, complementary nature of TGA and DTA, Applications of DTA in the study of clays, minerals, coals and explosives. Differential Scanning Calorimetry (DSC) – Principles, Methodology, Interpretation of DSC curves, comparison between DSC and DTA, chemical and pharmaceutical applications of DSC.

Unit-III Photo Chemistry:

**Unit-IV Non Equilibrium Thermodynamics:**

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager’s reciprocity relations, electro kinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

**Recommended books:**

Unit-I Synthetic methodology-I:
Introduction, Terms and definitions – Target molecule, Retrosynthesis, Disconnection, Synthon, Reagent, Transform and Synthetic equivalents. Criteria for selection of target molecule, Functional group interconversion (FGI), Disconnection or Synthon approach for organic synthesis, Synthetic tree, Linear and convergent synthesis. One-group C-X disconnections - Carboxylic acid derivatives (acid halides, esters, amides etc.), alcohols, ethers alkyl halides and sulphides. One-group C-C disconnections - Alcohols and carbonyl compounds, Retrosynthetic analysis involving chemo, regio and stereoselectivities.

Unit-II Synthetic methodology-II:
Introduction to Two-group C-C and C-X disconnections – Two-group C-X disconnections: 1,2-difunctionalised and 1,4-difunctionalised compounds with suitable examples. Two-group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised and 1,5-difunctionalised compounds - Michael addition and Robinson annulation. Control in carbonyl condensations (ex: Mevalonic acid). Rearrangements in synthesis strategy – Strategy in ring synthesis. Strategic bond approach, rules for Strategic bond approach, Application of the strategies to the synthesis of Multistriatin (+) Disparlure, and Longifolene.

Unit-III Stereoselective Synthesis-I:
Introduction, terminology and principles of stereoselective synthesis – Categories of stereoselective synthesis: Introduction to diastereoselective synthesis, enantioselective synthesis and double stereo differentiating reactions – Diastereomeric excess (de) and enantiomeric excess (ee). Strategies for stereo control in diastereoselective synthesis (preliminary conceptual treatment): Small ring templates, molecular walls, ring forming reactions pericyclic reactions, co-ordination metal centers, use of \(\pi\)-donor complexes, chiral auxiliaries, achiral auxiliaries, intra annular and extra annualr stereo control. Nucleophilic additions to cyclic and acyclic carbonyl compounds: Cram’s rule, Felkin’s model: addition to chelated carbonyl compounds, Prelog’s rule, addition to chelated carbonyl compounds, addition of –H and –R to cyclic ketones (Formation of axial and equatorial alcohols) Aldol reactions: (a) Achiral enolates with achiral aldehydes, (b) Achiral enolates with chiral aldehydes, (c) Chiral enolates with achiral aldehydes and (d)
chiral enolates chiral aldehydes.

**Unit-IV Stereoselective synthesis-II:**

Stereoselective transformation of C=C (double) bond: Diastereo selective synthesis involving catalytic hydrogenation, Hydroboration, Simmons-Smith reaction, Prevost reaction.

Enantioselective synthesis with chiral non racemic reagents: Hydroborations with chiral boranes; Reductions with chiral complex hydrides and chiral organometallic compounds.

Enantioselective synthesis with chiral non racemic catalysts: Catalysis by chiral transition metal complexes with reference to Sharpless enantioselective epoxidations and Jacobsen asymmetric epoxidations enantio selective hydrogenations. Enzyme mediated enantioselective synthesis.

Enantioselective Iminium catalyzed reactions- Diels – Alder reaction, Michael addition and 1,4-reduction of α, β-unsaturated aldehydes, Enamine asymmetric aldol reaction. Techniques for determination of enantiomeric excess- specific rotation and Chiral NMR.

**Recommended Books:**

1. Stereochemistry of organic compounds -Principles & Applications by D Nasipuri
2. Stereochemistry of Carbon compounds - Ernest L Eliel & Samuel H. Wilen
3. Stereochemistry: Conformation & Mechanism -P SKalsi
4. The third dimension in organic chemistry-Alan Bassendale
6. Asymmetric synthesis-Nogradi
7. Asymmetric organic reactions -J D Morrison and H S Moscher
9. Stereo differentiating reactions - Izumi
10. Enantioselective organocatalysis-Peter I Dallco
11. Organic Synthesis-The disconnection approach -S Warren
12. Organic Synthesis - C Willis and M Willis
13. Problems on organic synthesis - Stuart Warren
14. Organic synthesis-R. E. Ireland
15. Organic synthesis-Michael Smith
17. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
18. Organic synthesis by Michael B Smith
19. Some modern methods of organic synthesis - W Carruthers
Unit-I Electroanalysis methods:

Potentiometry – Theory of potentiometry, calculation of electrode potential at the equivalence point, Finding of equivalence volume – Linear and derivative titration plots, Ion-sensitive electrodes – Metal-based cation and anion sensitive electrodes, solid membrane electrodes, Glass electrodes, Liquid ion-exchange electrodes, Gas-sensing membrane electrodes.

Stripping voltammetry: Anodic stripping voltammetry, cathodic stripping voltammetry – Basic principles and applications.

Unit-II Spectrophotometry and Atomic absorption spectroscopy:


 Atomic absorption spectroscopy – Principles, Instrumentation, sources of radiation (Hollow cathode lamp and Electrodeless discharge lamp), Interferences and methods of minimization, Applications.

Unit-III Inductively coupled Plasma-related techniques and Molecular fluorescence spectroscopy:

Inductively coupled plasma-atomic emission spectroscopy (ICP-AES) and ICP-Mass spectrometry (ICP-MS) – Principles, Instrumentation, AES detectors, Quadrupole mass spectrometer, Difference between the two detectors, Applications in the analysis of trace and toxic metals in water, geological and industrial samples.

Molecular fluorescence spectroscopy – Principles, theory of fluorescence, phosphorescence, Relation between intensity of fluorescence and concentration, correlation of fluorescence with molecular structure, Fluorescence quenching, instrumentation, Applications.
Unit-IV Combined methods in structural characterization of compounds

Importance of structural characterization of compounds, selection and application of various methods in structural characterization of inorganic, coordination and organometallic compounds. Case studies of (1) Diborane (2) Ni(DMG)$_2$ (3) Ni(CO)$_4$ (4) [Co(en)$_2$F$_2$]$^+$ (5) Cu(Salen)$_2$ (6) Fe(CO)$_5$ (7) Fe$_2$(CO)$_9$ (8) Fe$_3$(CO)$_{12}$ (9) Ferrocene (10) [Cr(CH$_3$COO)$_2$.H$_2$O]$_2$

Recommended Books:

2) Principles of instrumental analysis, D.A. Skoog, F.J. Holler and T.A. Neiman, 5$^{th}$ ed., Harcourt Asia PTE Ltd.
5) Infrared and Raman spectra of inorganic and coordination compounds, K. Nakamoto.
6) Structural methods in inorganic chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Craddock, ELBS.
Unit-I  Organometallic Compounds –II:

Organometallic compounds of transition metals: Classification of transition metal organometallic compounds based on the nature of the ligands. \(^1\) bonded complexes of transition metals – Alkyls and aryls, types and routes of synthesis, stability and decomposition pathways, organocopper compounds in organic synthesis. Alkylidynes, alkylidyynes, low valent carbenes and carbines – synthesis, nature of bond, Structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit-II  Organometallic Compounds –III:

Organotransition metal compounds with –donor and –acceptor ligands – \(^2\), \(^3\), \(^4\) organic groups. Preparation, structures and properties of olefin complexes of iron and nickel groups Preparation, structures and properties of \(^5\)-allyl complexes of nickel and palladium complexes. Exo/endo conformers, \(^4\) –Butadiene complexes of cobalt, rhodium and iron. Organophosphines: Preparation and properties of organophosphines, organophosphines as ligands. Synthesis, structures and properties of organophosphine complexes of Rh and Pd.

Unit-III  Organometallic Compounds – IV:

Organotransition metal complexes of the cyclic n-perimeter: \(C_nH_n\): Preparation, Structure and reactions of – Fe, Co, and Ni complexes with cyclic \(^4\) \(C_4H_4(R_4)\) ligands. Fe, Ru, and Os complexes with \(^5\) (\(C_5H_5\)) ligands, Ti, V and Cr complexes with \(^6\) (\(C_6H_6\)) ligands and their carbonyl derivatives.

Organometallic compounds of lanthanides: Comparison of organometallic chemistry of \(d\)- and \(f\)-block metals. Homoleptic organolanthanides, cyclopentadienyl and pentamethyl cyclopentadienyl complexes of trivalent and divalent lanthanides – Structures and Applications in organic synthesis.

Unit-IV  Homogenous Catalysis:

Stoichiometric reactions for catalysis, catalytic reactions and the valence electron (16/18) rule, Oxidative addition reactions (H-H, H-X and R-X); Reductive elimination reactions: \(\square\)-and \(\square\)-elimination reactions and cyclometallation reactions. Asymmetric
hydrogenation; Olefin oxidation (Wacker’s process), Oligomerization & Polymerization (Ziegler-Natta Catalysis), Water gas shift reaction and Fischer-Tropsch reaction.

**Recommended books:**

1. Principles and applications of Organotransition metal chemistry, Collman.
2. The Organometallic chemistry of transition metals, Crabtree.
IV Semester - Inorganic Chemistry Practicals (Specialization)

Paper-V  Ion exchange and Solvent Extraction Methods  (4CHP13)
(Marks 100, 9 Hours per week)

Ion exchange and Solvent Extraction Methods

I. Ion exchange Methods
1. Determination of capacity of an anion exchange resin
2. Determination of capacity of a cation exchange resin
3. Separation and determination of Zinc and Magnesium using a cation exchange resin
4. Separation and determination of Chloride and Bromide using an anion exchange resin
5. Determination of the total cation concentration in a water sample.

II. Solvent Extraction Methods
1. Determination of Ni as anion NiDMG complex
2. Determination of Chloride ion and Iodide ion by AgNO₃
3. Determination of Pb as Pb-dithiazone complex

Paper-VI Instrumental Methods  (4CHP14)
(Marks 100, 9 Hours per week)

III. Analysis of Ternary mixtures
4. Ag⁺, Cu²⁺, and Ni²⁺
5. Cu²⁺, Ni²⁺ and Zn²⁺
6. Fe³⁺, Mg²⁺, and Ca²⁺

IV. Analysis of Complex materials
4. Brass
5. Devarda’s alloy
6. Cement

Recommended Books:
5. Comprehensive experimental chemistry - V.K. Ahluwalia, New publication

Scheme of Valuation
Marks 100  Time: 4Hours
Experiments (2)  80 Marks
Record/ Sample & Viva  20 Marks

Dean  Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
IV Semester-Organic specialization
Paper-III  General Organic Chemistry-II (4CHT21)
(Marks 100, Total Hours 60)

Unit-I  Heterocyclic Chemistry-III:
Methods of synthesis and reactivity of the following six membered heterocyclic systems:
Acridines, pyridazines, cinnolines, phthalazines, pyrimidines, quinazolines, pyrazines,
quinoxalines, - Structure determination and synthesis of uric acid and caffeine.

Unit-II Molecular Rearrangement in organic transformations:
Mechanisms and synthetic applications of rearrangement reactions- Beckmann
rearrangement, Curtius rearrangement, Hofmann rearrangement, Lossen rearrangement,
Schmidt rearrangement, Fries rearrangement, Wagner–Meerwein rearrangement, Wolff
Rearrangement, Baker-Venkataaraman Rearrangement, [1,2]-Wittig Rearrangement,
[2,3]-Wittig Rearrangement, Benzidine rearrangement Brook rearrangement and
Stevens’s rearrangement. Favorskii, Quasi-Favorskii Rearrangement.

Unit-III Chemistry of Vitamins and nonsteroidal hormones:
(a) Chemistry and synthesis of the following vitamins: A₁, A₂, B₁, B₂, B₆, H, K and C.
Chemistry and synthesis of non-steroidal hormones: Oxytocin, Thyroxin and Adrenalin.
Structure determination of Insulin (synthesis is not required).

Unit-IV Drugs:
Synthesis and pharmacological applications and adverse effects of Nifedipine, Acyclovir,
Warfarin, Fluconazole, Cefalexin, Sulfadoxine, Cycloserine, Chloroquine, Norfloxacin,
Levocetirizine, Sulfamethoxazole and Nateglinide.

Recommended Books
1. Bioorganic chemistry,- Herman Dugas
2. Organic Drug synthesis - Ledneiser Vol 1-6
3. Strategies for organic drug synthesis and design - Daniel Ledneiser
4. Top Drugs: Top synthetic routes - John Saunders
5. Organic chemistry - Vol. 1 and Vol. 2, Finar
6. March's Advanced Organic Chemistry - Michael B. Smith
7. Heterocyclic chemistry - R. K. Bansal
8. Heterocyclic Chemistry - T. Gilchrist

Dean Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
Unit-I  Chemistry of Flavanoids:
Classification of Flavanoids, General methods of synthesis of Anthocyanins, Flavones, Flavonols and Flavanones. Chemistry of Pelargonidin, Cyanidin, Delphinidin chloride, Chrysin, Quercitin and Diadzein.

Unit-II  Antibiotics:

Unit-III  Prostaglandins, Porphyrins and Carotenoids:

Unit-IV  Biosynthesis of Natural products:
Introduction, Major biosynthetic pathways: (a). Acetate hypothesis and its use in construction of Aromatic rings and Polyphenolic compounds (b). Mevalonic acid pathway-Ruzicka biogenetic isoprene rule, Biosynthesis of mono, sesqui and diterpenes – formation of the Presqualene alcohol and biosynthesis of triterpenes. (c) Shikimic acid pathway: Biosynthesis of essential amino acids (Phenyl alanine, Tyrosine and Tryptophan), Flavonoids, Porphyrins and Alkaloids (Morphine and Indole group alkaloids).

Recommended Books:
1. Biosynthesis - Geismann
2. Biosynthesis - Bernfeld
3. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
4. Organic chemistry - Vol. 2, Finar
IV Semester- Organic specialization
Paper IVB Medicinal chemistry (Elective-II) (4CHT22B)
(Marks 100, Total Hours 60)

Unit-I Basic concepts in Medicinal Chemistry:
Definition of Drug (WHO), Stereo chemical aspects of drugs, Classification of
drugs based on chemical structure, pharmacological action and mechanisms at molecular
level. Mechanism of drug action-Physical and Chemical action. Explanation of Quantal
dose, Graded dose, Efficacy, Potency, LD<sub>50</sub>, ED<sub>50</sub> Therapeutic index and Margin of
safety. Targets of Drug action: a) Receptors: Concept, Types of receptors, Agonist,
Antagonist, Partial and Inverse agonist. b) Ion channels c) Enzyme : Specific and non
specific Enzymes d) Carrier molecules.

Unit-II Drug Discovery:
1). a) Drug Discovery without Lead b) Lead discovery: Random screening, Non-random
screening and Drug metabolism studies. Clinical observations, Rational approaches to
Lead discovery.  2). Drug development: Lead modification- a) Identification of active part-
Pharmacophore b) Fundamental group modification c) Structure activity
relationship d) Structure modification to increase potency and therapeutic index i) Homologation ii) Chain branching iii) Ring chain transformations iv) Bioisoterism.
Drug development process: a) Pre-formulation and Product development. B) Preclinical
studies; Acute toxicity, Sub acute toxicity, Chronic toxicity, Mutagenecity and Reproductive studies c) Clinical Research: Phase –1, Phase –2 and Phase –3 d) Regulatory approval process. Cost of drug development.  3). Intellectual property in

Unit-III Pharmaco dynamic agents:
Definition, Mechanism of action at molecular level, synthesis, Medicinal uses and
Adverse effects of the following classes of compounds with special reference to specific
drugs mentioned under each class. 1) Anti-Inflammatory – Ibuprofen and NSAIDS. 2)
Anti-Emetic- Metoclopramide (5 HT-receptor antagonist). 3) Anti-Histamines –
Pheniramine and H1-Antagonist 4) Anti-Ulcer – Ranitidine, H2-Antagonist Omeprazole-
H<sup>+</sup>K<sup>+</sup>Atpase inhibitor. 5) Anti-Hypertensives: a) α-Blocker- Prozosine b) β-Blocker:-
Atenolol  c) Ca<sup>2+</sup> channel blockers- Nefedipine d) ACE-inhibitor - Enalapril e) Centrally
active - Methyl Dopa. 6) Anti-Anginal Drugs- Isorsorbide dinitrate  7) Bronchodilator-
Salbutamol. 8) Anti-Depressants- Fluxetine. 9). Drugs used in Schizophrenia -
Chlorpromazine  10) Anxiolytic-Sedative -Diazepam.
**Unit-IV Chemotherapeutic agents:**

**Recommended Books:**
2. Burger’s Medicinal Chemistry and Drug Discovery, Vol. 1-5, Wiley
3. Medicinal Chemistry, Ashutoshkar, New Age International Ltd
5. Essentials of Medical Pharmacology, K. D. Tripathi, Jaypee Brothers
8. A Text book of pharmaceutical chemistry, Jayasree Ghosh

Dean  
Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
**Paper-V Organic Chemistry practicals (4CHP15)**

(Marks 100, 9 Hours per week)

(A) **Estimations:**

1) Estimation of acetone /ethyl methyl ketone  
2) Estimation of aspirin  
3) Estimation of acid value  
4) Estimation of amino acid  
5) Estimation of unsaturation  
6) Estimation of glucose

(B) **Principles of chromatography:**

Determination of RF value – Ascending and descending techniques – Circular paper chromatography – Selection of solvents in paper chromatography – Location of spots in paper chromatography

Experiments in chromatography:

(a) Separation of leaf pigments – chlorophyll-‘a’ & ‘b’ xanthophylls

(b) Separation of amino acids by paper chromatography

(c) Determination of RF value of glycine by ascending paper chromatography

(d) Determination of various impurities by thin layer chromatography

(e) Purification of commercial anthracene by column chromatography using benzene

**Paper-VI Organic Chemistry practicals (4CHP16)**

(Marks 100, 9 Hours per week)

(A) **Isolation and purification of the following natural products:**

1) Caffeine 2) Embelin 3) Piperine 4) Lycopine 5) Nicotine 6) Rutin  
7) Lachnolic acid 8) Mangiferin

(B) **Advanced organic preparations:**

1) 2-methyl indole  
2) 2,5-dihydroxyacetophenone (Fries reaction)  
3) Photo-reduction of benzophenone  
4) Glucose to glucose penta acetate  
5) Ammonium thiocyanate to urea  
6) 1,2,3,4-Tetrahydrocarbazole.  
7) Antipyrin  
8) Benzocaine  
9) Benzimidazole  
10) Paracetamol

**Scheme of Valuation**

<table>
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<tr>
<th>Marks 100</th>
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<td>Experiments (2)</td>
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Dean

Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
IV Semester-Physical chemistry specialization
Paper III Catalysis (4CHT23)
(Marks 100, Total Hours 60)

**Unit-I Heterogeneous Catalysis:**

**Unit-II Phase-Transfer catalysis:**
Classification , characteristises and criterion for P.T.C.catalysis. Mechanism and types of P.T.C catalysed reactions. Preparation of P.T.C.catalysts like quaternary salts, tetrahexyl ammonium bromide and crown ethers.Application to hydrolysis, oxidation, reduction, esterification and formation of ethers. 

**Metal ion catalysis:** Molecular activation, proximity, interaction and catalytic cycle. Application to hydrogenation, isomerization, oxidation and hydroformylation.

**Micellar catalysis:** Micellization and types of surfactants-critical micellar concentration(CMC)and its determination-factors effecting CMC. Solubilization in surfactant solutions. Emulsion polymerization mechanism.

**Unit-III Acid-Base Catalysis:**

**Anchord catalysis:** Concept of anchored catalysis and types. Montemorillorite anchored catalysis and its reactions.

**Unit-IV Enzyme Catalysis:**
inhibition. Enzymatic catalytic mechanism by Acid-base catalysis, Covalent catalysis, Metal ion catalysis, Catalysis through proximity and orientation effects, catalysis by preferential transition state binding.

**Recommended books:**
6. Organicmetallic Chemistry-R.C. Mehrothra
7. Biochemistry, Voet and Voetjohn Wiely
8. Catalysis-J.C.Kuriacose-Macmillan-India Ltd.
IV Semester-Physical chemistry specialization
Paper IV(A)- (Elective-I)
Nanomaterials, Macromolecules and Data analysis (4CHT24A)
(Marks 100, Total Hours 60)

**Unit-I Nanoparticles and their applications:**

**Unit-II Characterization of Macromolecules:**

**Unit-III Kinetics –IV:**

**Unit-IV Data Analysis:**
Types of errors, Accuracy and precision, methods of expressing them. Least square analysis-average and standard deviations, correlation coefficient Normal (Gaussian) distribution, significant figures, comparison of results Student t-test, F-test, Chi square test. Dipole moments and its measurements. Its application to molecular structure determination. Phase rule and its derivation. Application of phase rule to three component systems.

Dean Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
**Recommended books:**

2. Nanochemistry, G.B. Sergeev, Elsevier
4. Principles of polymerization - George Odian (John Wiley)
6. Quantitative Inorganic Analysis, A.I. Vogel
7. Polymer Chemistry, B. Vollmert.
IV Semester-Physical chemistry specialization
Paper IV(A)- (Elective-II) (4CHT24B)

Supramolecular, Material Sciences, Lasers and Computational Chemistry
(Marks 100,Total Hours 60)

Unit-I: Supramolecular Chemistry:

Unit-II Types of materials and liquid crystals:

Unit-III Lasers in Chemistry:
**Unit-IV Computational Chemistry:**


**Recommended books:**

5. Principal of Physical chemistry by Puri & Sharma.
6. Molecular Modelling: Principles and Applications by AndrewLeach,Longman publications
7. Computational chemistry,GuyH.Grant & W.GrahamRichards,OxfordUniversity press.
11. Lasers in Chemistry and Biological Sciences,S.Chopra & H.M.Chawla,Wiley Eastern Ltd
IV Semester-Physical chemistry Practicals

Paper-V Kinetics experiments (4CHP17) (Marks 100, 9 Hours per week)

1. Kinetics of
   i) Actone- Iodine reaction: Determination of
      a) Order       b) Acid effect
      c) Solvent effect   d) Temperature effect.
   ii) Inversion of sucrose-Effect of acidity functions.

Paper–VI Instrumentation (4CHP18)
(Marks 100, 9 Hours per week)

Instrumentation:

I. Conductometry:
   1. Mixture of acids and CuSO₄ vs NaOH
   2. Dibasic acids Vs NaOH
   3. Mixture of chloroacetic acids vs NaOH
   4. Replacement Reactions
   5. Determination of pKₐ of chloroacetic acid
   6. Verification of Onsagers euations with KCl
   7. Determination of composition of complex (Cu(II) Vs EDTA)

II. Potentiometry /pH Metry:
   1. Determination of dissociation constants of moaobasic / dibasic acids by Albert-Serjeant method.
   2. Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane.
   3. Determination of thermodynamic constans, ΔG, ΔS and ΔH for the following reaction by e.m.f. method.
      \[ \text{Zn} + \text{H}_2\text{SO}_4 \rightarrow \text{ZnSO}_4 + 2\text{H} \]

III. Polarography:
   1. Estimation of Pb²⁺, Cd²⁺ and Ni²⁺ separately and in a complex.

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Dean  
Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
Recommended books:

2. Practical physical chemistry - B. Vishwanthan and P.S. Raghavan.
3. Practical physical chemistry - B.D. Khosla and V. C. Gard, R. Chand or Co. Delhi.
4. Systematic experimental physical chemistry - S.W. RajBhoj and Dr. T.K. Chondhekar

Prof. Gade Dayakar
Chairperson
Board of Studies in Chemistry
Kakatiya University - Warangal

Mobile: +91- 9849777797
Email: gadedayakar@yahoo.co.in

Dean

Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
Model paper

M.Sc CHEMISTRY

Internal examination

Scheme of examination:

**Internal examination**: [Best of 2 – Internal exam-I, Internal exam-II]

In each exam – No. of questions – 10    Total marks – 20    Duration of exam – 1Hr

(Internal exam-I from Unit I and Unit II; Internal exam-II from Unit III and Unit IV)

Dean

Prof. Gade Dayakar, Chairperson, BOS in Chemistry, KU,
MODEL PAPER

FACULTY OF SCIENCE
M.Sc (-Semester examination)

CHEMISTRY

Time: 3Hrs Paper- Max Marks: 80

*Answer ALL questions in serial order*
All questions carry equal marks

1. Answer the following (4x4=16M)
   a) Unit-I
   b) Unit-II
   c) Unit-III
   d) Unit-IV

2. a) Unit-I (16M)
   b) Unit-I
   c) Unit-I
   d) Unit-I
   Or

3. a) Unit-II (16M)
   b) Unit-II
   c) Unit-II
   d) Unit-II
   Or

4. a) Unit-III (16M)
   b) Unit-III
   c) Unit-III
   d) Unit-III
   Or

5. a) Unit-IV (16M)
   b) Unit-IV
   c) Unit-IV
   d) Unit-IV
   Or

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