DRAVIDIAN UNIVERSITY

KUPPAM – 517426

A.P, INDIA

M.Sc. CHEMISTRY (Organic)

(SELF SUPPORTING)

CURRICULUM

(EFFECTIVE FROM THE ACADEMIC YEAR 2020-21)

DEPARTMENT OF CHEMISTRY

(School of Herbal Studies and Naturo Sciences)

ACADEMIC REGULATIONS FOR
M.Sc. Chemistry (2 YEAR PROGRAMME)

Name of the Programme: **M.Sc. Chemistry (Organic)**

A brief description of the programme: This programme is two years full-time course to impart knowledge and training in different branches of Chemistry so as to equip them for seeking jobs in industries and in research and is also comes under the School of Herbal Studies and Naturo Sciences.

Board of Studies: The Board of Studies in Chemistry has approved the contents of the syllabi of I, II, III & IV semesters of M.Sc. Chemistry (Organic Chemistry) programme Under CBCS System and also recommended books for the courses on 26th November 2019.

Contents of Programme

1) Core courses – Compulsory,
2) Internal Elective Courses – Open for the students of the particular programme in which they are admitted,
3) External Elective Courses – Open for the students from the other departments,

Eligibility to M. Sc. Chemistry (Organic) Programme: B. Sc, Degree with chemistry or industrial chemistry with any of the two of the following, Mathematics'/Botany/Physics/Geology/Zoology/Biochemistry/Microbiology/Biotechnology/ Sericulture/Instrumentation/Chemical technology.

- Selection of candidates through entrance examinations.

Credits (Theory, Practicals, Core and Electives): 100 credits,

Core papers : 74 credits
Internal Electives (IE) : 16 credits
External Electives (EE) : 6 credits (2 EE X 3= 06 credits)
Soft skills: 4 credits (2 SS X 2 = 4 credits)

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100 Credits
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Number of Semesters, : 4 **Semesters**

Distribution of courses : 1st Semester: 24 credits – 600 Max Marks
2nd Semester: 25 credits – 600 Max Marks
3rd Semester: 25 credits – 600 Max Marks
4th Semester: 26 credits – 650 Max Marks

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100 Credits 2450 Max Marks
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Scheme of Instructions:

The scheme of instructions shall be for a duration of 2 academic years, each consisting of 2 semesters i.e., 4 semesters for M. Sc. programme. The department shall offer a minimum two internal electives in a semester. A course in external elective shall be offered by a department only when there is a minimum enrolment of three students for that particular course. One credit shall mean one period of teaching for theory or two periods for laboratory per week in a semester for 90 working days (15 weeks).

Syllabus

The Choice Based Credit System (CBCS) was introduced in all Departments of the University From the academic year (2013-2014). According to this system the M.Sc. Chemistry (Organic) Programme requires a student to earn 100 credits in four semesters. The basic programme structure and the scheme of examinations are as follows.

M. Sc., CHEMISTRY (Organic) -- CBCS SEMESTER SYSTEM

(EFFECTIVE FROM THE ACADEMIC YEAR 2020--21)

PROGRAMME STRUCTURE

The two-year M.Sc., Chemistry (Organic Chemistry) programme will have four semesters.

The Programme structure will be as given below:

Paper No.	Title of the Paper	Type of Paper	Periods/ Week	Duration of Exam (Hours)	IA	EA	Maximum Marks	Credits
I Semester								
CHM 101	Inorganic Chemistry	Core	4	3	30	70	100	4
CHM 102	Organic Chemistry	Core	4	3	30	70	100	4
CHM 103	Physical Chemistry	Core	4	3	30	70	100	4
CHM 104	General Chemistry & Computers for Chemists	Core	4	3	30	70	100	4
Practical								
CHM 105	Inorganic Chemistry	Core	5	3	-	-	67	3
CHM 106	Organic Chemistry	Core	5	3	-	-	67	2.5
CHM 107	Physical Chemistry	Core	5	3			66	2.5
Total Marks and Credits for I Semester							**600**	**24**
II Semester								
CHM 201	Inorganic Chemistry	Core	4	3	30	70	100	4
CHM 202	Organic Chemistry	Core	4	3	30	70	100	4
CHM 203	Physical Chemistry	Core	4	3	30	70	100	4
CHM 204	Chemistry of Consumer Products	EE	3	3	20	40	60	3
		SS	2	3			40	2
Practical								
CHM 205	Inorganic Chemistry	Core	5	3			66	2.5
CHM 206	Organic Chemistry	Core	5	3			67	3

CHM 207	Physical Chemistry	Core	5				67	2.5
Total Marks and Credits for II Semester							**600**	**25**
III Semester								
CHM 301	Spectroscopy and its Applications	Core	4	3	30	70	100	4
CHM 302	General Chemistry	Core	4	3	30	70	100	4
CHM 303	A. Polymer Chemistry/ B. Nano Chemistry	IE	4	3	30	70	100	4
CHM 304	Chemistry and Environment	EE	3	3	20	40	60	3
		SS	2	3			40	2
Practical								
CHM 305	Spectral Identifications of Organic Compounds	Core	6	4			100	4
CHM 306	IE Practical	IE	6	4			100	4
Total Marks and Credits for III Semester							**600**	**25**
IV Semester (A)								
CHM 401	Organic Synthesis –I	Core	4	3	30	70	100	4
CHM 402	Organic Synthesis –II	Core	4	3	30	70	100	4
CHM 403	A. Heterocyclic Chemistry/ B. Drug Chemistry	IE	4	3	30	70	100	4
CHM 404	A. Natural Products / B. Bio Organic Chemistry	IE	4	3	30	70	100	4
Practical								
CHM 405	Multistep Synthesis of organic compounds	Core	6	4			100	4
CHM 406	Estimations of Organic Compounds	Core	6	4			100	4
	Seminar	Core			50		50	2
Total Marks and Credits for IV Semester							**650**	**26**
Grand Total Marks and Credits for 4 Semesters							**2450**	**100**

OR

IV Semester (B)								
CHM 401	Organic Synthesis –I	Core	4	3	30	70	100	4
CHM 402	Organic Synthesis –II	Core	4	3	30	70	100	4
CHM 403	Dissertation	IE	16			200	200	8
Practical								
CHM 404	Multistep Synthesis of organic compounds		6	4			100	4
CHM 405	Estimations of Organic Compounds		6	4			100	4
	Seminar				50		50	2
Total Marks and Credits for IV Semester							**650**	**26**
Grand Total Marks and Credits for 4 Semesters							**2450**	**100**

DRAVIDIAN UNIVERSITY

M.Sc. CHEMISTRY SYLLABUS, UNDER (CBCS)

FIRST SEMESTER

CHM 101: INORGANIC CHEMISTRY

UNIT-I: Coordination Compounds 15 Hrs

Introduction to Crystal field Theory, CFSE, and its calculation, Paring energy, Splitting of 'd' orbital's in Octahedral, Tetrahedral and square planar geometries, John –Teller effect, Distortion in tetragonal and square planar crystal fields Application of CFT, Shortcomings of CFT, Evidence for covalency –Nephelauxetic effect. MOT of co-ordinate bonds – M.O. Diagrams for octahedral and tetrahedral. Spectrochemical series, Isomerisation, Racemization.

UNIT-II: Metal-Ligand equilibria in solution 15 Hrs

(i). Metal-ligand equilibria in solution Stepwise and overall formation constants and their interrelationship, Trends in stepwise formation constants, factors affecting the stability of metal complexes, Chelate effect, Determination of binary formation constants by pH-metry and spectrophotometric methods.

(ii). Theory of Hard Soft Acid-Base (HSAB)

Hard and soft acids and bases, Classification, Acid-Base strength and hardness, Symbiosis, Electronegativity and hardness, Application of HSAB: Biological functions, toxicology of metals, and medicinal applications.

UNIT – III: Transition Metal π- Complexes 15 Hrs

Transition metal π – complexes with unsaturated organic molecules – alkenes, alkynes, diene, dienyl, and Cyclo Penta dienyl complexes and arene complexes-general methods of preparation, properties, nature of bonding and structural features – Important reactions relating to Nucleophilic and Electrophilic attack on ligands and to organic synthesis.

UNIT-IV: (A). Carbonyl and nitrosyl complexes 15 Hrs

Preparation of Metal Carbonyls of Mn, Fe, Co and Ni, Bonding in Carbonyls, EAN in Carbonyls, terminal and Bridging Carbonyls, Structures of mononuclear, binuclear, trinuclear. Metal nitrosyls and chemistry of linear and bent nitrosyls, nitrosyls as NO^+ and NO^-, Analytical uses of nitrosyl complexes.

(B). Metal atom clusters

Higher boranes, Carboranes, metal-metal bonds in carbonyl cluster, LNCCs and HNCCs, Isoelectronic and Iso label relationships, Heteroatom in metal atom clusters, electron counting schemes for HNCCs, HNCCs of Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, and Pt.

Books Suggested:

1. Inorganic Chemistry by J. E. Huheey, E.A. Keiter and R.A. Keiter, 4th edition, Harper Collins, 1993.
2. Advanced Inorganic Chemistry by F.A. Cotton, G. Wilkinson, C.A. Murillo, and M. Bochmann, 6th edition, Wiley Inter science N.Y, 1999.
3. Coordination Chemistry by F. Baisalo and R. Johnson (WA Benjamin Inc).,1964.
4. Inorganic Chemistry, Principles, and Applications by I.S. Butler and I.F. Harper, Benjamin Cummings, Redwood City, CA, 1989.
5. Chemistry of Complex equilibria, M. T. Beck, Von Nostrand Reinhold, London,1990.
6. Metal Complexes in aqueous solutions, A. E. Martell and R.D. Hancock, Plenum Press New York.,1996.
7. Mechanism of Inorganic Reactions by F. Baisalo and R. G. Pearson, 2nd Edn.,
8. Concise Inorganic Chemistry by J. D. Lee, 4th edition, ELBS, 1994.
9. Chemistry of Elements by N. N. Greenwood, Pergamon press.
10. Organometallic chemistry by R.C Malhotra and A. Singh.
11. Inorganic Chemistry: G. Wolfsburg (University Science Books)
12. Modern Inorganic Chemistry W. L. Jolly, 2nd Ed. (Mc Graw-Hill).
13. Coordination Compounds. S. F. Kettle (Springer).

CHM 102: ORGANIC CHEMISTRY

UNIT—I: Nature of bonding in Organic molecules and Aromaticity 15 Hrs

Nature of Bonding in Organic Molecules and Aromaticity, Delocalized chemical bonding conjugation, cross conjugation, resonance, hyper conjugation, tautomerism, Huckle's rule and the concept of aromaticity, aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, metallocenes - Ferrocene, Azulenes, Fulvenes, Annulenes, anti-aromaticity, pseudo-aromaticity, homo-aromaticity.

UNIT - II: Stereochemistry 15 Hrs

Chiral point group classifications of stereo isomers based on symmetry and energy considerations- Dissymmetric and asymmetric molecules. Molecules with tetra-coordinate chiral center (quaternary ammonium salts, N-oxide, silane derivatives, phosphines, and sulfones). Molecules with tri-coordinate chiral center (tertiary amines, carbanions, phosphines, and sulphoxide). Concept of dynamic enantiomerism. Molecules with two or more chiral centers, Constitutionally unsymmetrical molecules (with dissimilar chiral carbons) and constitutionally symmetrical molecules (with similar chiral carbons), Principles of axial Chirality, Stereochemistry of allenes, spiranes and biphenyls. Geometrical isomerism in molecules having C=C, C=N, N=N and in cyclo propane's, cyclo butanes & cyclo pentane, E, Z nomenclature, Physical, spectral and chemical methods of determining E, Z configuration.

UNIT- III: Reactive Intermediates and Molecular Rearrangements 15 Hrs

Reactive intermediates - Generation, Structure, and stability of (i). carbocations, (ii). carbanions, (iii). carbenes, (iv). nitrenes and (v). free radicals. Molecular rearrangements: Definition & Classification, Molecular rearrangements involving (i). Electron-deficient carbon Wagner-Meerwein, Pinacol-Pinacolone and Wolf rearrangements. (ii). Electron deficient nitrogen; Hoffman, Lossen, Curtis, Schmidt and Beckmann rearrangements. (iii). Electron deficient oxygen Baeyer-villiger oxidation Base catalyzed rearrangements, Benzilic acid rearrangement, Favorskii rearrangement, Trans annular and Sommlett-Hauser rearrangement.

UNIT-IV: Substitution Reactions 15 Hrs

i). Aliphatic Nucleophilic substitutions: A brief review of Nucleophilic Substitution Reactions at saturated carbons. S_N1, S_N2, and S_Ni- mechanisms and stereochemistry – Factors affecting the rate of S_N1 and S_N2 reactions such as substrate structure, nature of leaving group, nucleophile and the solvent. Neighboring group participation: Definition, Criteria of determining neighboring group participation (enhanced reaction rates, retention of configuration, isolation of cyclic intermediates and isotopic labeling) Examples of neighboring group participation involving halogens, oxygen, sulfur, nitrogen, aryl, cyclo alkyl groups with σ and π-bonds. Introduction to non-classical Carbonium ions.

ii). Aromatic Nucleophilic Substitution: The S_NAr, S_N1, benzene, and $S_{RN}1$mechanisms. Reactivity - effect of substrate, structure, leaving group and attacking nucleophile. The von Richter, Sommelet - Hauser, and Smiles rearrangements.

Reference Books

1. Stereochemistry of carbon compounds by Ernest L. Eliel.
2. Stereochemistry by V. M. Potapov.
3. Stereochemistry of organic compounds – principles and applications by D. Nasipuri.
4. Stereochemistry, Conformation, and Mechanism by P. S. Kalsi.
5. The third dimension in organic Chemistry by Alan Bassindale.
6. Organic Chemistry by T. J. Salmons.
7. Organic Chemistry by Robert T. Morrison and Robert N. Boyd.
8. A guide book to mechanism in Organic Chemistry by Peter Sykes.
9. Advanced Organic Chemistry: Reactions, Mechanism & Structure by Jerry March.
10. Reactive Intermediates by Isaac.
11. Mechanism and structure in Organic Chemistry by S. Mukherjee.
12. Name Reactions by Jie.
13. Advanced Organic Chemistry, F.A. Carey and R. J. Sundberg, Plenum.
14. Structure and Mechanism in Organic Chemistry C. K. Ingold, Cornell University Press.
15. Principles of Organic Synthesis, R.O.C Norman and J. M. Coxon, Blackie Academic.
16. Stereochemistry, P. S. Kalsi, Wiley Eastern.
17. Textbook of Organic Chemistry, M. C. Murry.
18. Organic Chemistry, Vol I, I. L. Finisar, ELBSEds.

CHM 103: PHYSICAL CHEMISTRY

UNIT – I: Quantum Chemistry -I **15 Hrs**

Introduction to Heisenberg Principle, de Broglie theorem, wave function, condition for normalization and orthogonality. Algebra of operators, linear and non-linear operators. Commutation, Eigen functions, and Eigen values. Postulates of Quantum mechanics Quantum mechanical solution of some model systems viz particle in one-dimensional box particle in three-dimensional box, one-dimensional harmonic oscillator rigid rotator, Quantum number. Separation of variables. Application to hydrogen and hydrogen-like atom. Graphical representation of orbital's.

UNIT – II: Chemical Dynamics **15 Hrs**

Methods of determining rate laws, Collision theory of reaction rates, Steric factor, Activated complex theory, Arrhenius Equation, Treatment of uni molecular reactions, Lindemann, Lindemann – Hinshelwood. Dynamic chain, hydrogen-bromine reaction, Pyrolysis of acetaldehyde, decomposition of ethane, photochemical reactions-hydrogen-bromine, hydrogen- chlorine reactions, Autocatalysis, hydrogen-oxygen reaction, explosion limits.

UNIT – III: Thermodynamics-I **15 Hrs**

(A). Classical Thermodynamics

Basic concepts of laws of thermodynamics, free energy, chemical potential and entropy, partial molar properties: their significance and determination of partial molar volume, fugacity, and determination.

(B). Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable Distribution, Ensemble averaging, Postulates of ensemble averaging, canonical, grand canonical and micro-canonical ensembles, partition functions, translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions, Heat capacity, chemical equilibria and equilibrium constant in terms of partition functions, Entropy of monatomic gases (Sackur-Tetrade equation).

UNIT – IV: Electrochemistry - I **15 Hrs**

(A). Thermodynamic and Kinetic concept of Electrochemistry

Thermodynamic and Kinetic Derivation of Nernst Equation, Chemical and Concentration Cells with and without Transference, Liquid Junction Potential, Derivation of the Expression for Liquid Junction Potentials-its determination and elimination, Applications of EMF Measurements: (i)Solubility product, (ii) p^H Determination, (iii) Potentiometric Titrations.

(B). Conductivity

Theory of Electrolytic Conductance, Derivation of Debye-Huckle Equation and its Verification, Debye-Falkenhagen Effect, and Wein Effect, kohlrausch law. Calculation of Solubility of Sparingly Soluble Salt from Conductance Measurements.

Conductometric Titrations :

i). Titration of Strong Acid Vs Strong Base (HCl vs NaOH).

ii). Titration of Weak Acid Vs Strong Base.

iii). Titration of mixture of Strong and Weak Acids vs Strong Base.

iv). Precipitation Titrations.

Books Suggested:

1. Physical Chemistry, P. W. Atkins (ELBS).
2. Introduction to Quantum Chemistry, A. K. Chandra (Tata Mc Graw Hill).
3. Quantum Chemistry, Ira N. Levine (Prentice Hall).
4. Chemical Kinetics, K.J. Ladler (McGraw Hill).
5. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose (McMillan).
6. Thermodynamics for Chemists, S. Gladstone.
7. Chemical Thermodynamics, I. M. Klotz.
8. Statistical Thermodynamics, M. Dole.
9. Modern Electrochemistry, vol. I & II, J. O. M. Bockris and A. K. N. Reddy (Plenum).
10. An Introduction to Electrochemistry (3rd ed.), S. Glantone (An affiliated East-West).

CHM 104: General Chemistry & Computers for Chemists

UNIT – I: Symmetry and Group Theory **15 Hrs**

Symmetry Elements and Symmetry operation, Definitions of a group, sub-group, Relation between orders of a finite group and its sub-group, Conjugacy Relation and classes-point symmetry group, Schonflies symbols, Representation of groups by matrices (representation for C n9 C nv9 D nh9 etc. groups to be worked out explicitly), character of a representation. The great orthogonality theorem (without proof), Character tables.

UNIT-II: Errors and Data Handling **15 Hrs**

Introduction of Errors and data handling, Classification of errors, precision and accuracy, mean and median values, Standard deviation, Minimization of errors, Distribution of random errors, Confidence interval, Comparison of results, student's t-test, F-test, Comparison of means of two samples and more than two samples (ANOVA), Correlation and regression, Significant figures, Linear-least-square fitting.

UNIT-III: Thermal Methods and Radio Analytical Methods **15 Hrs**

Thermal Methods: Thermogravimetry –Principle, Factors affecting the results, instrumentation. Application with special reference to $CuSO_4 5H_2O$, $CaC_2O_4\ 2H_2O$. Different thermal analysis – principle, instrumentation, difference between Thermo Gravimetry (TG) and Differential Thermal Analysis(DTA), applications with special reference to the clays and minerals. Different scanning calorimetry –principle, and applications to inorganic materials like chlorates and per chlorates, ammonium nitrate.

Radio analytical Methods: Definition and measurement of radioactivity. Devices G.M counter and scintillation counter. Radioactive tracers. Typical applications of radioisotopes as tracers. Principle and applications of Isotope dilution technique and Activation analysis.

UNIT – IV: Introduction to Computers and Computing **15 Hrs**

(A). Introduction:

Basic Structure and functioning of computers with a PC as an illustrative example. I/O devices, Memory, Secondary Storage, Computer languages, Operating Systems, Introduction to Windows, Introduction to Algorithms and Flow –charts.

(B). Computer Programming in C Language:

C Language Fundamentals, the characters set. Identifiers and keywords, data types – constants and variables, declarations, expressions, and operators. Data Input and output, Control Statements, Functions and Arrays.

Books Suggested:

1. H.W. Willard, LL. Merritt and J. A. Dean: Instrumental Methods of Analysis

2. Vogel's Textbook of Quantitative Inorganic Analysis.

3. Instrumental Methods of Analysis H. Kaur.

4. Micelles, Theoretical and applied aspects, V. Moroi (Plenum)

Books Suggested for Computers:

1. Computer and Common Sense, R. Hunt and J. Shelly (Prentice Hall).

2. An Introduction to Digital Computer Design, V. Raja Raman and T. Radha Krishna (Prentice Hall).

3. Computational Chemistry, A. C. Norris.

4. Microcomputer Quantum Mechanics, J. P. Killngbeek and Adam Hilger.

I SEMESTER PRACTICAL SYLLABUS

105: Inorganic Chemistry Practicals

I. Semi-Micro Qualitative analysis of mixture containing four cations of rare elements Rare Elements:- W, Te, Se, Mo, Zr, Ce, Th, V and Li Insoluble's:- $PbSo_4$, $SrSo_4$, Al_2O_3, Cr_2O_3, Fe_2O_3, SnO_2, TiO_2, ThO_2, WO_3.

II. Preparations:-

a. Cis-Potassium tri(oxalate) Ferrate (III) trihydrate
b. Hexaminine Cobalt (III) Chloride
c. Tris Thiourea Zinc (II) Sulphate

106: Organic Chemistry Practicals

I. Systematic qualitative analysis of organic compound (Acid, Base, Phenol, Aldehyde,

Ketone, Ester, Hydrocarbon, Carbohydrate) and preparation of their Derivatives.

107: Physical Chemistry Practicals

1. Determination of Critical solution Temperature of phenol water system study of the effect of electrolyte on CST.
2. Determination of Eutectic composition and Temperature of the binary system (Urea – benzoic acid)
3. Determination of rate constant of acid hydrolysis of an Ester and investigating the effect of catalyst concentration and Temperature.
4. Verification of Langmuir adsorption isotherm. Determination concentration of acetic acid by studying its absorption on charcoal,

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SECOND SEMESTER

CHM 201: INORGANIC CHEMISTRY

UNIT – I: Organometallic chemistry **15 Hrs**

(A). Organo-metallic reagents in synthesis

Stoichiometric reactions in catalysis, homogeneous catalytic hydrogenation, hydro formylation, (oxo reaction), isomerization, Zeigler-Natta polymerization of olefins, oxopalladation reactions, Activation of small molecules by coordination.

(B). Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as η^2 -olefin, η^3-allyl, and dienyl complexes.

UNIT-II: Reaction mechanisms in complexes **15 Hrs**

Reactivity of metal complexes, Inert and labile complexes, Kinetics and mechanisms of substitution reactions, Kinetics of substitution reactions in octahedral complexes, Acid hydrolysis, Factors affecting acid hydrolysis, base hydrolysis, Conjugate base mechanism, Anation reactions, Substitution reactions in square planar complexes, Trans effect, theories and applications of trans effect, Electron transfer reactions, Inner sphere and outer sphere mechanisms, Marcus theory.

UNIT – III: Electronic Spectra of Complexes **15 Hrs**

Frank–Condon principle, Russel–Saunders coupling, Spectroscopic term symbol, Multiple terms of excited states (microstates), selection rules, Break down of selection rules, spin-orbit coupling, Band Intensities, Orgel Diagrams for d^1 to d^9 configurations. Tanabe-Sugano Diagrams, Spectra of octahedral complexes of metal ions in aqueous media like Ti^{3+}, Cu^{2+}, V^{3+}, Ni^{2+}, Cr^{3+}, Co^{2+}, Cr^{2+}, Fe^{2+}, and Mn^{2+} , Spectra of spin paired configurations of Mn^{3+}, Mn^{2+}, Fe^{3+}, Fe^{2+} and Co^{2+} , Spectra of Tetrahedral complexes of Mn^{2+}, Co^{2+}, Cu^{2+} and Ni^{2+}, Calculation of Dq and B parameters, Charge transfer spectra.

UNIT – IV: Bioinorganic chemistry **15 Hrs**

A: Essential and trace metals, the role of metal ions in biological systems, Na+/K+ pump, Bioenergetics, and Adenosine Tri Phosphate (ATP) Cycle, Deoxy Nucleic Acid (DNA) polymerization, glucose storage, chlorophylls, photo system I and photo system II in cleavage of water.

B: Oxygen and electron transportation in biological systems

Heme proteins and oxygen uptake, structure and functions of hemoglobin Myoglobin hemocyanin and hemerythrin structure and functions of metallo proteins in electron transfer process, cytochromes, and iron-sulfur proteins.

Books Suggested:

1. Inorganic Chemistry Principles of Structure and Reactivity 6th Edition. James. E. Huheey.

2. Organometallic Chemistry: R.C. Malhotra and Singh.

3. R.S. Drago: Structural Methods in Inorganic Chemistry.

4. Advanced Inorganic Chemistry [5th Edition] F.A. Cotton and G. Wilkinson, John Wiley.

5. Molecular spectroscopy, Banweel.

6. Concise Inorganic Chemistry [5th Edition] J. D. Lee [Black Well].

CHM 202: ORGANIC CHEMISTRY

UNIT- I: Reaction Mechanism **15 Hrs**

Determination of reaction mechanism, Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediate, use of isotopes, chemical trapping, cross over experiments, Use of IR and NMR in the investigation of the reaction mechanism.

a) Addition to carbon-carbon multiple bonds- Addition involving symmetrical and unsymmetrical reagents, Addition of halogens to alkenes, evidence for halonium ion intermediacy, stereoselectivity and specificity, *Syn. addition reagents* like $KMnO_4$, OsO_4, Anti addition – Epoxidation followed by ring-opening.

b) Elimination reactions: E_2, E_1, E_1CB mechanisms. Orientation and stereo selectivity in E_2 elimination reactions. Pyrolytic *syn*. elimination and α elimination. Elimination vs. substitution.

UNIT – II: Pericyclic Reactions **15 Hrs**

Characteristics --- Types of Pericyclic reactions – Electro cyclic, cycloaddition – cyclo reversion and sigma tropic reactions-examples – 4n and 4n+2 electron type – stereo-specificity. Theories involved in understanding Pericyclic reactions.

(a).Frontier Molecular Orbital Theory concept – Woodward – Hoffmann selection rules for electro cyclic, cycloaddition—cyclo reversion and sigma tropic reactions based on FMO approach. Examples.

(b). Conservation of Molecular Orbital's Theory concept – Framing of Woodward – Hoffmann selection rules for electro cyclic, cycloaddition and cyclo reversions based on conservation of Molecular Orbital's approach.

(c).Aromatic Transition state Theory – concept – Woodward- Hoffmann selection rules for electro cyclic reactions, cycloaddition-cyclo reversions and sigma tropic reactions based on ATS aromatic transition state (Huckel-Mobius) approach. Examples.

Unit-III: Conformational Analysis **15 Hrs**

Introduction to conformational isomerism and the concept of dynamic stereochemistry, Study of conformations in ethane and 1,2-disubstituted ethane derivatives like butane, di halo butane halo hydrin, ethylene glycol, butane-2,3-diol, amino alcohols, and 1,1,2,2-tetrahalobutanes. Klyne-Prolog terminology for conformers and torsion angles. Conformations of unsaturated acyclic compounds (1-butene, propio naldehyde, and butanone). Conformational dia stereo isomers and conformational Enantiomers. Factors affecting the conformational stability and conformational equilibrium-attractive and repulsive interactions. Use of physical and spectral methods in conformational analysis.

Conformational effects on the stability and reactivity of acyclic dia stereo isomers-steric and stereo electronic factors-examples. Conformation and reactivity. The Weinstein-Holness equation and the Curtin-Hammett principle. Conformations of cyclo hexanes, mono, and di-substituted cyclo hexanes. Stereochemistry of decalins. Factors governing the reactivity of axial

and equatorial substituents in cyclo hexanes. Stereochemistry of addition to the carbonyl group of the rigid cyclo hexane ring.

UNIT-IV: Organic Photochemistry – II **15 Hrs**

Norrish cleavages, type I: Mechanism, acyclic cyclic diones, influence of sensitizer, photo Fries rearrangement. Norrish Type II cleavage: Mechanism and stereochemistry, type II reactions of esters: 1:2 di ketones, photo decarboxylation. Photochemistry of unsaturated ketones – Olefin photochemistry, cyclic olefins – Photochemistry – of conjugated dienes; electro cyclization, influence of triplet energy of sensitizer, sensitized and unsensitized electro cyclization. Electro cyclization of dienes in crossed sense – Photochemistry of benzene derivatives – formation of derivatives of benzavalene, fluvene, and Dewar benzene, cycloaddition of benzene to olefins and dienes – Decomposition of nitrites – Barton reaction. Di-π methane rearrangement.

References:

1. Conservation of orbital symmetry by Woodward and Hoffmann.
2. Organic reactions and orbital symmetry by Gilchrist and Storr.
3. Pericyclic reactions—a problem-solving approach by Lehr and Merchand.
4. Pericyclic reactions by Mukherjee.
5. Mechanism and structure in organic chemistry by S, Mukherjee.
6. Some modern methods of organic synthesis by W. Carothers.
7. A guide book of organic synthesis by R. K. Mackie, D. M. Smith & R. A. Atken.
8. Reagents in organic synthesis by B. P. Munday and others.
9. Organic synthesis by O. House.
10. Organic synthesis by Michael B. Smith.
11. Reagents for organic synthesis by Fieser & Fieser, Vol. 1-11(1984).
12. Handbook of reagents for organic synthesis by Reich and Rigby Vol. I &IV.
13. Organic Synthesis by Robert Ireland.
14. The third dimension in organic chemistry by Alan Bassindale.
15. Stereochemistry of carbon compounds by Ernest L. Eliel.
16. Stereochemistry of Organic compounds- Principles and Applications by D. Nasipuri.
17. Stereochemistry, Conformational, and Mechanism By P. S. Kalsi.
18. Heterocyclic chemistry, T. L. Gilchrist, Longman UK Ltd., London (1985).

CHM 203: PHYSICAL CHEMISTRY

UNIT – I: Quantum Chemistry II **15 Hrs**

(A). Angular momentum

Ordinary Angular momentum, Generalized Angular momentum, L and L operators of angular momentum, operator using Ladder operator, addition of angular momenta, Spin, anti symmetry and Pauli Exclusion Principle, Slater determinant.

(B). Electronic Structure of Atoms

Russel-Saunders coupling, degeneracy, Term symbols, term separation energies of pn and dn configurations, spin-orbit coupling and Zeeman splitting.

(C). Molecular Orbital Theory

Huckle theory of conjugated systems, π-bond order and charge density calculations, application to ethylene, butadiene and benzene.

UNIT – II: Chemical Kinetics **15 Hrs**

Effect of a substituent on the rate of reaction-Hammett's and Taft's equation, use of and constants and extended Hammett equation.

Acid-Base catalysis: Homogenous acid-base catalysis-mechanism of acid-base catalysis, protolytic and prototropic mechanism.

Enzyme catalysis: Specification and classification of enzymes, Kinetics, and mechanism of single substrate reaction, Michael-Menten kinetics, production, detection, and estimation of free radicals.

UNIT-III: Thermodynamics-II **15 Hrs**

(A). Phase Equilibria:

Equilibrium between two phases of one component. The Clapeyron equation. The Clausius Clapeyron equation. Applications. The integrated form of the Clapeyron equation.

(B). Phase rule: Thermodynamic derivation of phase rule, Solid-liquid equilibria, Thermal analysis, simple eutectic, congruent fusion, incongruent fusion, and systems consisting of both. Application of phase rule to the three-component system, Stokes and Roozeboom plots. Three-component liquid systems, formation of one pair, two pairs and three pairs of partially miscible liquids, two salts, and water, no chemical combination, double salt formation, one salt forms hydrate and two salts form hydrates, solid solutions.

UNIT – IV: Electrochemistry- II **15 Hrs**

(A). Irreversible Electrode Phenomenon

Reversibility and irreversibility, Dissolution and deposition potentials, Decomposition voltage, overvoltage, diffusion overvoltage, charge transfer overvoltage, reaction overvoltage,

concentration overvoltage, and phase overvoltage and hydrogen and oxygen over voltages, Tafel plots, Exchange current density and Transfer coefficient, Butler-Volmer equation for one-electron transfer processes.

(B). Polarography

Theory of Polarography, diffusion current, Ilkovice equation, Equation for half-wave potentials for reversible system when oxidant alone, reductant alone and both are present.

Books Suggested:

1. Physical Chemistry, P. W. Atkins, (ELBS).

2. Introduction to Quantum Chemistry, A. K. Chandra (Tata McGraw Hill).

3. Quantum Chemistry, Ira N. Levine, (prentice Hall).

4. Coulsons's' Valence, R. Mcweeny, (ELBS).

5. Modern Electrochemistry, vol. I & II, J. O. M. Bockris and A. K. N. Reddy (Plenum).

6. An Introduction to Electrochemistry (3rd ed.), S. Glasstone (Affiliated East-West).

7. Micelles, theoretical and applied aspects, V. Moroi (Plenum).

8. A Text-Book of Physical Chemistry (2nd Ed.), S. Glasstone (Macmillan).

9. Principles of Physical Chemistry, Maron and Prutton.

10. Theoretical Electrochemistry, L. I. Antropov.

CHM-204 CHEMISTRY OF CONSUMER PRODUCTS (EXTERNAL ELECTIVE)

UNIT 1: Soaps **15 hrs**

Saponification of oils and fats. Manufacture of soaps. Formulation of toilet soaps. Different ingredients used. Their functions. Medicated soaps. Herbal soaps. Mechanism of action of soap. Soft soaps. Shaving soaps and creams. ISI specifications. Testing procedures/limits.

UNIT 2: Detergents **15 hrs**

a. Anionic detergents: Manufacture of LAB (linear alkyl benzene). Sulphonation of LAB – preparation of acid slurry. Different ingredients in the formulation of detergent powders and soaps. Liquid detergents. Foam boosters. AOS (alpha olefin sulphonates.
b. cationic detergents: examples. Manufacture and applications.
c. Non-ionic detergents: examples. Manufacture of ethylene oxide condensater.
d. Mechanism of action of detergents. Comparison of soaps and detergents. Biodegradation environmental effects. ISI specifications / limits.

UNIT 3: Shampoos **15 hrs**

Manufacture of SLS and SLES. Ingredients. Functions. Different kinds of shampoos – anti-dandruff, anti-lice, herbal and baby shampoos. Hair dye. Manufacture of conditioners. Coco betaines or coco di ethanolamides – ISI specifications. Testing procedures and limits.

UNIT 4: Skin preparations **15 hrs**

Face and skin powders. Ingredients, functions. Different types. Snows and face creams. Chemical ingredients used. Anti per spirants. Sunscreen preparations. UV absorbers. Skin bleaching agents. Depilatories. Turmeric and Neem preparations. Vitamin oil. Nail polishes: nail polish preparation, nail polish removers. Article removers. Lipsticks, roughs, eyebrow pencils. Ingredients and functions – hazards. ISI specifications. GMP – ISO 9000/12000 – consumer education. Evaluation of the product – advertisements.

Reference books

1. Gopala Rao. S, Outlines of chemical technology, Affiliated East-West Press,1998.

2. Kafaro, Wasteless chemical processing, Mir publishers, 1995.

3. Sawyer. W, Experimental cosmetics, Dover Publishers, New York, 2000.

II SEMESTER PRACTICAL SYLLABUS

205: Organic Chemistry Practicals

I. Systematic qualitative analysis of unknown organic mixture containing two components

i. Acid + Neutral

ii. Base + Neutral

iii. Phenol + Neutral

iv. Neutral + Neutral

206:Physical Chemistry Practicals

I. Conductometry

a. Titration of a Strong acid with Strong base

b. Titration of a Weak acid with Strong base

c. Determination of cell constant

II. Potentiometry

a. Titration of a Strong acid with Strong base

b. Titration of a Weak acid with Strong base

c. Redox Titrations

207: Inorganic Chemistry Practicals

I Complexometric Titrations

a) Determination of Mg^{+2}g by using EDTA

b) Determination of Zn^{+2} by using EDTA

II Quantitative Separation and Determination of the following pairs of metal Ions using Complex metric Titrations.

a) Separation of Iron Determination of Nickel Fe^{+2} and Ni^{+2}.

b) Separation of Copper Determination of Zinc Cu^{+2} and Zn^{+2}.

c) Separation of Copper Determination of Nickel Cu^{+2} and Ni^{+2}.

III. Determination of Metal Ions using colourmetric methods

a. Estimation of Manganese

b. Estimation of Nickel

c. Estimation of Iron

THIRD SEMESTER

CHM 301: SPECTROSCOPY AND ITS APPLICATIONS

UNIT -I: UV - Visible Spectroscopy, ORD & CD 15 Hrs

UV and visible spectroscopy: Various electronic transitions (185-800nm), the effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-wood ward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. The steric effect in biphenyls.

ORD: α-Axial halo ketone rule and octant rule – Application of these rules in the determination of absolute configuration of cyclohexanones, decalones, and cholestanones.

Circular Dichroism : Principle – positive and negative cotton effects – Absolute configuration.

UNIT -II: IR Spectroscopy 15 Hrs

IR Spectroscopy: Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols, and amines. The detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FT-IR.

UNIT –III: ^{1}HNMR spectroscopy 15 Hrs

Nuclear spin, nuclear resonance, Saturation shielding of magnetic nuclei, chemical shifts and its measurements, factors influencing chemical shift, deshielding. Spin-spin interactions, factors influencing coupling constants 'J' classification (ABX, AMX, ABC, A_2B_2, etc.), spin decoupling, basic ideas about instrument, FT-NMR, advantages of FT-NMR.

Applications of ^{1}H NMR : Shielding mechanism, mechanism of measurement , chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (First order spectra), virtual coupling, Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear over Hauser effect (NOE).

^{13}C NMR Spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbon), coupling constants.

UNIT -IV: Mass Spectrometry **15 Hrs**

Introduction, principle, instrumentation, single and double-focusing mass spectrophotometer, Ionization Methods EI, CI, FD, FAB, Factors affecting fragmentation ion analysis, ion abundance, Molecular-ion peak, Nitrogen rule, Base peak, Meta stable ion, Isotopic abundance, Mc Lafferty rearrangement. Mass spectral fragmentation patterns of various classes of organic compounds, Alkanes, cyclo alkanes, alkenes, aromatic hydrocarbons, Aliphatic, Aromatic, Aldehydes, Ketones, Alcohols, phenols, aliphatic Aromatic Nitro Compounds Nitrites, Nitrates, Nitriles.

REFERENCE BOOKS:

1. Electron Spin Resonance Elementary Theory and Practical Applications- John E. Wertz and James R. Bolton, Chapman and Hall, 1986.
2. Spectroscopic Identification of organic compounds – Silverstein, Bassler, and Morril.
3. Organic Spectroscopy- William Kemp.
4. Fundamentals of Molecular Spectroscopy- C.N. Banwell and E.A. Mc cash 4th Edition, Tata Mc Graw Hill Publishing Co., Ltd.1994.
5. Physical Methods in Inorganic Chemistry – R. S. Drago, Saunders Publications.
6. Application of Mossbauer Spectroscopy – Green Mood.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in inorganic chemistry – R.V Parish, Ellis, Harwood.
8. Instrumental Methods of Chemical Analysis- H. Kaur, Pragati Prakashan, 2003.
9. Instrumental Methods of Analysis, 7th Edition – Willard, Merit, Dean, Settle, CBS Publications, 1986.
10. Molecular Structure and Spectroscopy – G. Arul has, Prentice Hall of India Pvt. Ltd, New Delhi, 2001.
11. Mossbauer Spectroscopy – N.N. Green-Wood and T.C. Gibb, Chapman, and Hall, Landon1971.
12. Coordination Chemistry: Experimental Methods - K. Burger, London Butter Worth's, 1973.
13. Analytical spectroscopy – Kamlesh Bansal, Campus books, 2008.
14. Structural Inorganic Chemistry Mossbauer Spectroscopy –Bhide.
15. Principle of Mossbauer Spectroscopy – T.C. Gibb, Chapman, and Hall, Landon 1976.

CHM 302: GENERAL CHEMISTRY

UNIT – I: Electron Spin Resonance Spectroscopy **15 Hrs**

Basic Principles and Instrumentation of ESR

g and A tensors and Interpretation of g values, Relaxation Process and line width in ESR transitions, Interaction between nuclear spin and electron spin, Hyperfine Coupling, Spin polarization for atoms and transitional metal ions, factors affecting g values, Application to transition metal complexes having one unpaired electron and to inorganic free radicals, Zero field splitting, Kramer's degeneracy and its applications.

UNIT – II: Mossbauer and NQR Spectroscopy **15Hrs**

(A) Mossbauer Spectroscopy

Basic principles, spectral parameters and spectrum display, Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin (2) Sn^{2+} and Sn^{4+} compounds, nature of M-L bond, coordination number and in equivalent MB atoms.

(**B) Nuclear Quadrupole Resonance Spectroscopy**

Basic principles of NQR spectroscopy, Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting and applications.

UNIT – III: Chromatography **15 Hrs**

Principles of analytical separation: Plate theory, Rate theory, Craig concept of counter current distribution, process optimization, retention analysis, resolution (fundamental equation). Gas Chromatography, Liquid Chromatography (Including high performance Chromatography), Ion exchange Chromatography, separation of actinides by ion exchange resins, Ion Chromatography, Size Exclusion Chromatography, Planar Chromatography (PC, TLC, HPTLC), Reverse phase Chromatography and Bonded phase Chromatography (BPC), Super critical Fluid Chromatography.

UNIT-IV: A. Photo Electron Spectroscopy **15 Hrs**

Introduction, Principles, Instrumentation theory, application and comparison with other methods, Auger electron spectroscopy electron Spectroscopy for chemical Analysis- Principles and applications.

B. Atomic Absorption Spectroscopy: Introduction, Principles, Relation between emission and absorption, and band width, Instrumentation, Interferences, back ground correction, accuracy precision,

sensitivity and detection limits. Applications, indirect determination of AAS elements, special consideration to chromium, Be, Hg, Mo, analysis of water Analytical

Books Suggested:

1. Magneto-chemistry, R. L. Carlin (Springer-Verlag).

2. Elements of Magneto chemistry, R. L. Dutta and A. Syamal (Affiliated East-West).

3. Molecular Spectroscopy, Banwell.

4. Instrumental Methods of Analysis, H. W. Willard, L. L. Merritt and J. A. Dean (Affiliated East-West).

5. Vogel's Text Book of Quantitative Analysis J. Bassett, R. C. Denny, G. H. Jeffery and J. Mendham (ELBS).

6. Principles of Instrumental Analysis, D. A. Skoog and D. M. West (Holt, Rinehart and Wilson).

7. Analytical Chemistry, J. G. Dick (McGraw Hill).

8. Basic principles of Spectroscopy, R. Chang (Mc Graw Hill).

9. Analytical chromatography – G.R. Chatwal, Himalaya publishing House, VII Edition

10. Instrumental Methods of Analysis By Willard. Merit and Dean 7th Edition.

11. Spectroscopy by Chatwal and Anand, Himalaya Publishing House.

12. Basic principles of Spectroscopy R. Chang [McGraw Hill]

CHM 303 - POLYMER CHEMISTRY (INTERNAL ELECTIVE)

UNIT-I: Basic concepts in Polymer Chemistry **15 Hrs**

Introduction of Monomers, Polymers, Repeat units, Functionality, Degree of Polymerization (Dp) and High Polymers.

Classification of Polymers: Thermo plastics and Thermosets, Plastics Elastormers, Fibers, Homo & Co-Polymers.

Polymerization Types: Addition, Condensation, Co-ordination and Co-polymerization. Polymerization Techniques: Bulk, Solution, Suspension and Emulsion Polymerization.

UNIT-II: Polymer Characterization **15 Hrs**

Concept of Average molecular weight, Polydispersity and its significance in polymers. Number average (M_n), Weight average (M_w), Viscosity average (M_v) and Z-average (M_z), and Molecular weight distribution. Determination of molecular weight averages by and End group analysis, Osmometry, Viscosity, Gel permeation chromatography (GPC), Light scattering, and Ultracentrifugation methods. Sedimentation velocity method and Testing of polymers.

UNIT-III: Physical Properties of Polymers and Polymer Solutions **15 Hrs**

Glass Transition Temperature:

Definition, Determination of 'Tg' and factors influencing on Tg. Crystallinity: Degree of Crystallinity and Polymer Crystallization behavior. Rheology of Polymer Materials: Hooke's equation, Newton's equation; Maxwell models for Visco-Elasticity; Deformation behavior polymers.

Polymer Solutions: Process of Polymer dissolution; Thermodynamics of polymer dissolution. Flory-Huggins theory of polymer solutions.

UNIT-IV: Polymer Processing **15 Hrs**

Polymers processing by Extrusion Technique. Injection molding & Blow molding methods. Fiber spinning: Spinning process – melt, Dry and wet spinning.

Books Suggested:

1. Text Book of polymer science by Gowarikar, Sreedhar, and Viswanathan, Wiley-Eastern Publications. India.
2. Introduction to polymers – by R. J. Young, Chapman, and Hall, U. K.
3. Organic polymer chemistry by K. J. Saunders, 2nd Ed., Chapman Hall Publications, U.K., 1988.
4. Plastic materials by J. Brydson, 7th ed., Butterworth-Heineman, Elsevier (2005).
5. Polymer processing by D.H. Morton Jones, Chapman, and Hall, UK.
6. Polymer Processing and Fundamentals: Tim A Ostwald, Hansar publications.

CHM 303 - NANO CHEMISTRY (INTERNAL ELECTIVE)

UNIT-I: Basics of Nano chemistry **15 Hrs**

Introduction, physico – Chemical properties of Nanomaterials and Nanostructures in nature, Self-assembly – materials & molecules, Self Assembled Monolayers (SAM) and soft lithography, Nano wires and Nano machines. Techniques used in nano chemistry.

UNIT-II: Nanoparticles & Nanocomposites **15 Hrs**

Introduction, Types of Nanoparticles, pure metals – Gold, Silver & Cobalt, Metal Oxides – Silica, Iron Oxide Alumina & Titania; Synthesis of Nanoparticles, Characterization of Nanoparticles, Applications & Significance of Nano Particles. Introduction- polymer as matrix, Nylons, Polystyrene, Epoxy resins Nanomaterials as fillers – Nano fiber and Nano clays; Fabrication and processing of composites, Applications of Nanocomposites.

UNIT-III: Nanomaterials **15 Hrs**

Definition – Synthesis of Dendrimers – Divergent and Convergent methods – Structures, properties and applications of Dendrimers. Synthesis & purification of fullerenes – Chemical properties & Nano chemistry of fullerene. Carbon Nanotubes: Structural aspects, Properties of Carbon Nanotubes – Chemical, Mechanical and Electromagnetic properties, Carbon Nanotubes as transistors, as fibers and films.

UNIT-IV: Nanomaterials Synthesis **15 Hrs**

Introduction to Synthesis Strategies – Synthesis of Materials based on solubility principles – sol-gel Techniques – Templates based synthesis – micro emulsion Techniques – Electrochemical synthesis – Newer synthetic strategies for Nanomaterials from Laboratory & Industry.

Books Suggested:

1. Nanomaterials & Nano Chemistry, C. Breechigneae, P. Houdy, M. Lahmai (Eds.) Springer 2007.
2. Nano Chemistry G.B. Sergeev, Elsevier.
3. Nano Chemistry: A Chemical approach to Nano Materials, G.A. OZIN & A.C Arse Nault RSC publishing.
4. B. Viswanathan. Synthetic Strategies in Chemistry NCCR press (2008).
5. G. Schmidt Nanoparticle from Theory to Applications Wiley-VCH (2004).

CHM 304 –CHEMISTRY AND ENVIRONMENT (EE)

UNIT-I: Energy and Environment **15 Hrs**

Types of energy:- (Conventional and Non-Conventional) - Green energy (solar, tidal, wind, hydrothermal and geothermal). Biomass and its application. Nuclear energy (Fusion and Fission).

UNIT-II: Air Pollution **15 Hrs**

Classification and properties of air pollutants – emission sources – major emissions from global sources – the importance of anthropogenic sources behavior and fate of air pollutants – photochemical smog – effects of air pollution – health vegetation – material damage in India, control methods for air pollution. Vehicular air pollution; Air pollution from Portland cement plant – steel mills and petroleum refineries.

UNIT-III: Soil Pollution **15 Hrs**

Introduction – Soil pollution by Industrial wastes, by Urban wastes and radioactive pollutants. Agricultural practices – chemicals & metallic pollutants – Biological agents – mining – Detrimental effects of soil pollutants – effects of industrial pollutants –effects of modern agro-technology – Diseases caused by soil pollution – solid waste management.

UNIT-IV: Water Pollution **15 Hrs**

Introduction – Types of water pollutants. Sewage and domestic wastes – Industrial wastes – Agriculture discharges – toxic metals. Disease-causing agents – soils – detergents and phosphates. Analysis of water – DO, BOD, COD, & Hardness. Wastewater treatment (Advanced) – Removal of Suspended oils and Dissolved solids.

Books Suggested:

1. Environmental Chemistry by W. More & J. More.

2. Environmental Chemistry by S.S. Dara.

3. Environmental Chemistry by A. Sharma.

4. Environmental Chemistry by A. K. De.

5. Henry C Perkins (1974) Air Pollution, Mc Graw-Hill.

6. Kudesia, V.P. (1985) Water Pollution, Pragati Prakashan.

7. Engineering chemistry by Jain & Jain.

8. Industrial chemistry by B.K. Sharma.

III SEMESTER PRACTICAL SYLLABUS

305: Spectral Identification of Organic Compounds

Spectroscopy:

Identification of organic compounds by the analysis of their spectral data/spectra (U.V, I.R, PMR, CMR, and MS).

306: Polymeric Materials

a. Estimation of Monomer.
b. Determination of the Viscosity average Molecular weight of a Polymer by viscometer method.
c. Identification of polymers by physical and chemical means.
d. Synthesis of polymers
e. Degradation studies of Poly (Vinyl alcohol) by Viscosity method.

FOURTH SEMESTER

CHM 401 - ORGANIC SYNTHESIS – I

UNIT -I: Organo Phosphorous and Organo Sulphur Compounds 15 Hrs

Properties of divalent sulphur and trivalent phosphorous derivatives, nucleophilic reactivities, hard and soft acids and bases, compounds containing phosphorous-oxygen bonds, the phosphoroyl group, molecules with hydrogen-bonded to phosphoroyl group, Arbusov reactions, Perkov reactions, compounds containing sulphur-oxygen bonds, sulphoxide and sulfones-Pummerer rearrangements, sulphoxide as oxidizing agents, phosphorous ylides, Wittig's reactions and mechanism, the Emmons-Wadsworth reaction, reactions of sulphur ylides.

UNIT -II: New synthetic reactions 15 Hrs

(i) Protecting Groups: (a). Protection of alcohol by ether, silyl ether, and ester formation.

(b). Protection of 1, 2-diols by acetal, ketal and carbonate formation (c). Protection of amines by Acetylation, benzoylation, benzyloxy carbonyl, t-butyl oxy carbonyl, fmoc, and tri phenyl methyl groups, (d). Protection of carbonyls by acetal, ketal, and thiol acetal (Umpolung) groups,

(e). Protection of carboxylic acids by ester and ortho ester (OBO) formation.

(ii) Baylis-Hillman reaction, RCM olefin metathesis. Stork-enamine reaction and Umpolung use of di thio acetals.

Unit-III: Reagents of Synthetic Importance (Oxidations Reductions) 15 Hrs

(a) Oxidations: (i). Alcohols to carbonyls: Cr (VI) oxidants, Swern oxidation, Silver Carbonate.

(ii). Prevost and Woodward oxidation. (iii). Oxidations of allylic and benzylic C-H bonds: DDQ and SeO_2.

(b) Reductions: (i). Catalytic hydrogenation: Homogeneous hydrogenation-Use of Wilkinson's catalyst. (ii). Dissolving metal reductions including Birch reduction. (iii). Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$, and their modifications. Electrophilic metal hydrides: BH_3, and AlH_3. (iv). Hydrogenolysis, use of tri-n-butyl tin hydride.

(c) Organometallic Reagents: Preparation and application of the following in organic synthesis :

(i) Organo lithium and Organo copper reagents. (ii). Organo boranes in C—C bond formation.

UNIT -IV: Synthetic Strategies 15 Hrs

Synthetic Strategies, Terminology: target, synthon, synthetic equivalent, functional group inter conversion (FGI), functional group addition, functional group elimination. Criteria for selection of target. Linear and convergent synthesis. Retro synthetic analysis and synthesis involving

chemo selectivity, region selectivity, reversal of polarity and cyclization. Strategic bond: Criteria for disconnection of strategic bonds. Importance of the order of events in organic synthesis. One group and two group C-X disconnections. One group C-C disconnections. Alcohol and carbonyl compounds. Two group C-C disconnections; Diels Alder reaction, 1,3- di functionalized compounds, Control in carbonyl condensation, 1, 5- di functionalized compounds, Michael addition, and Robinson annulations, synthesis of (+) Di sparlure by retro synthetic approach.

Recommended Books:

1. Some modern methods of organic synthesis by W Caruthers.
2. Guidebook to organic synthesis, by R K Mackie, DM Smith & R A Atken.
3. Organic synthesis by O House.
4. Organic synthesis by Michael B Smith.
5. Reagents for organic synthesis, by Fieser & Fieser, Vol1-11(1984).
6. Organic synthesis by Robert EIreland.
7. Organic Synthesis - The disconnection approach by S. Warren.
8. Organic Synthesis by C Willis and M Willis.
9. Handbook of reagents for organic synthesis by Reich and Rigby, Vo I, IV.
10. Problems on organic synthesis by Stuart Warren.
11. Total synthesis of natural products: the Chiron approach by S. Hanessian.
12. Organic chemistry Calydon and others 2005.
13. Name Reactions by Jie Jack Li.
14. Reagents in Organic synthesis by B.P. Mundy and others.
15. Tandem Organic Reactions by Tse-LokHo Ho.
16. Advanced Organic Chemistry-Reactions and Mechanism, 2nd Ed. By Bernard Miller and Rajendra Prasad (Pages 397-414).

CHM 402 - ORGANIC SYNTHESIS – II

UNIT –I: Asymmetric Synthesis-I 15 Hrs

Introduction and terminology: Topocity in molecules Homotopic, stereo heterotopic (enantiotopic and diastereotopic) groups and faces- symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re, and Si. Selectivity in synthesis: Stereo specific reactions (substrate stereoselectivity). Conditions Stereo selective reactions (product stereoselectivity): Enantio selectivity and dia stereoselectivity.: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing Enantio and dia stereoselectivity. Analytical methods: % Enantiomer excess, optical purity, % diastereomeric excess. Techniques for determination of Enantio selectivity: Specific rotation, Chiral ^{1}H NMR, Chiral lanthanide shift reagents and Chiral HPLC.

UNIT -II: Asymmetric Synthesis-II 15 Hrs

Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2- asymmetric induction, Cram's rule, and Felkin-Anhmodel.

i) Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral Enolates, azaenolates, 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder and Aldol reactions.

ii) Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric Hydroboration using IPC2 BH and IPCBH2.Reductions with CBS reagent.

iii) Chiral catalyst controlled asymmetric synthesis: Sharpless, Jacobsen and Shi asymmetric epoxidations. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyoricatalysts, Enzyme mediated Enantio selective synthesis:

UNIT-III: Organometallic Reagents 15 Hrs

Synthesis and applications of Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium and Rhodium compounds in Organic Synthesis, Homogeneous catalytic hydrogenation and hydro formylation reactions.

UNIT IV: Methods of Polymerization (Synthetic Polymers) 15 Hrs

Reactions-Addition and condensation polymerization processes- Bulk, Solution, Suspension and Emulsion polymerization. Stereo specific Polymers-Preparation and significance- classification of polymers based on physical properties-Thermoplastics-Thermosetting plastics-Fibers and Elastormers - General applications. Preparation of Polymers-Preparation of Polymers based on different types of monomers. Industrial applications-olefin polymers-Diene polymers-nylons-Glyptal resins-Urea-formaldehyde, phenol-formaldehyde, and melamine resins- Epoxy resins - Ion exchange resins.

Recommended Books:

1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. The third dimension in organic chemistry, by Alan Bassendale
3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. Stereochemistry of Carbon compounds by Ernest Eliel
5. Stereo selectivity in organic synthesis by R S Ward.
6. Asymmetric synthesis by Nogradi.
7. Asymmetric organic reactions by Morrison and HS Mosher.
8. Stereo differentiating reactions by Izumi.
9. Some modern methods of organic synthesis by W Caruthers.
10. Guidebook to organic synthesis, by R K Mackie, DM Smith & R A Atken.
11. Organic synthesis by Michael B Smith.
12. Molecular Reactions and Photochemistry by Depuy and Chapman.
13. Photochemistry by C W S Wells.
14. Organic Photochemistry by Turro.
15. Molecular Photochemistry by Gilbert & Baggo.
16. Organic Photochemistry by D Coyle.

CHM 403 A - HETEROCYCLIC CHEMISTRY (INTERNAL ELECTIVE)

UNIT – I: Nomenclature of Heterocycles **15 Hrs**

Hantzsch-Widman system of nomenclature for monocyclic, fused and bridged Heterocycles. Three and Four Membered Heterocycles - Synthesis and reactions of aziridines, oxiranes, thietanes, azetidines, oxetanes, and thietanes.

UNIT – II: Five-Membered Heterocycles **15 Hrs**

Synthesis and reactions of pyrazole, imidazole, oxazole, Thiazole, Isoxazole and Iso thiazoles.

UNIT – III: Benzo fused Five-Membered Heterocycles **15 Hrs**

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans, benzothiophenes, and Benzimidazoles.

UNIT – IV: Six Membered Heterocycles **15 Hrs**

With one Heteroatom: Synthesis and reactions of Tetra hydro pyridine, pyran and thiopyran. With two or more Hetero atoms: Synthesis and reactions of diazines, and triazines.

Books Suggested:

1. Heterocyclic Chemistry Vol.1-3, R. R. Gupta, M. Kumar, and V. Gupta, Springer Verlag.

2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.

3. Heterocyclic Chemistry, J. A. Joule, K. Kills and G. F. Smith, Chapman, and Hall.

4. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Technical.

5. Contemporary Heterocyclic Chemistry, G. R. Newkome, and W. W. paudler. Wiley inter-Science.

6. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.

7. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, eds. Pergamon Press.

8. Principles of Modern Heterocyclic Chemistry, L. A. Paquette.

9. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, ELBS.

10. Advanced Organic Chemistry: Reactions and mechanisms, Bernard Miller.

CHM 403 B- PHARMACEUTICAL CHEMISTRY (INTERNAL ELECTIVE)

UNIT-I: Basic Principles of Pharmacology **15 Hrs**

i. Introduction, definitions Pharmacokinetics (ADME) Routes of drug administration Absorption, distribution, metabolism, and excretion of drugs, Bioavailability.
ii. Pharmacodynamics, Principles of drug action, Theories of drug action (Occupancy theory, rate theory, induced-fit theory, and macromolecular perturbation theory). Mechanism of drug action, Drug Synergism, and antagonism Drug toxicity.

UNIT-II: Drug Design and Lead Modifications **15 Hrs**

Introduction, Lead discovery, Lead modifications, structure pruning techniques taking morphine (naturally occurring alkaloid) as a pharmacophore. Uses of physicochemical properties in drug, designing like Lipophilic barrier to drugs p^{ka}, p^{H} Partition theory Ionization. Bio-isosterism and its applications. QSAR methods and parameters in drug designing Prodrug, classification of prodrugs, preparation of prodrugs. Design of prodrugs to improve the physical and biological properties of drug.

UNIT-III: Drugs Acting on Autonomic Nervous system (ANS) and Cardiovascular System (CVS).

15 Hrs

Organization and Basic Physiology of ANS and CVS - Definition, Classification, Nomenclature, Structure, Mode of action and Synthesis of Selected Drugs. Drugs Acting on Autonomic Nervous System Sympathomimetics and Sympatholytics – Definition, and examples of receptors, agonists, antagonists and neurotransmitters Epinephrine (Adrenaline), Norepinephrine (Noradrenalin), salbutamol, propranolol. Parasympathomimetics and parasympatholytics – Acetylcholine, Neostigmine Neuromuscular Junction Blocking Agents – Succinylcholine, d-tubocurarine, decamethonium.

Drugs Acting on Cardio Vascular System
Antihypertensive drugs – Methyl dopa
Antianginal drugs – Iso so sorbide dinatrate and Nitroglycerine,
Anti arrhythmic drugs – Quinidine,

B). Drugs acting on Ion channels and membranes – Nifedipine.
C). Angiotensin-Converting Enzyme Inhibitors – Captopril, Enalapril.

UNIT – IV: Drugs Acting on Central Nervous System **15 Hrs**

Organization and Basic Physiology of the Central Nervous System. Neurohumoral transmission in the CNS.

I). Nonsteroidal, Antipyretics, analgesics and anti-inflammatory agents-Paracetamol, Aspirin, Ibuprofen, Steroidal anti-inflammatory agents-Betamethasone.

Psychopharmacological drugs-Chlorpromazine.

Anti Parkinsonism drugs-Levodopa. Tranquilizers-Diazepam.

Books Suggested:

1. Medicinal Chemistry and Pharmaceutical Chemistry – Hari Kishan Singh and Kapur.
2. Medicinal Chemistry and Bio-Chemistry R. L. Nath.
3. Introduction to Medicinal Chemistry, Patric.
4. Berger's Medicinal Chemistry Vols. 1-5, -Manfred E. Wolf.
5. Comprehensive Medicinal Chemistry Vols. 1-5 Hauzsch.
6. Introduction to drug design, Silverman.
7. A biochemical approach to Medicinal Chemistry, Thomas Nogrady.
8. Principles of Medicinal Chemistry, William Foye.
9. Textbook of Organic medicinal and pharmaceutical chemistry-Delgado and William A.
10. The Organic Chemistry of Drug Synthesis Vols. 1-6-Ledneicer Top drugs top synthetic routes – John Saunders.
11. Medicinal Chemistry, Ashutoshnkar.
12. Synthetic Organic Chemistry and drugs, "Gurdeep & Chetwal"
13. Practical Pharmaceutical Chemistry, Becket & Stalls.

CHM 404 A: CHEMISTRY OF NATURAL PRODUCTS (I E)

UNIT – 1: Terpenoids **15 Hrs**

Occurrence, isolation, general methods of structure determination, isoprene rule, special isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Camphor, Farnesol, Zingiberene, Cadinene.

UNIT – II: Alkaloids **15 Hrs**

Occurrence, isolation, general methods of structure elucidation and physiological action, degradation, classification based on nitrogen heterocyclic ring, structure, stereochemistry, synthesis and biosynthesis of the following: Morphine, Strychnine, and Reserpine

UNIT – III: Steroids **15 Hrs**

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination, and synthesis of Cholesterol (total synthesis not expected), Androsterone, Testosterone, Estrone, Progesterone,

UNIT – IV: Flavonoids, Iso flavonoids and Prostaglandins **15 Hrs**

(A). Flavonoids, Iso flavonoids: Occurrence, nomenclature and general methods of structure determination, Isolation and synthesis of Apigenine, Luteolin, Quercetin, Biosynthesis of flavonoids and Iso flavonoids: Acetate Pathway and Shikimic acid Pathway.

(B). Prostaglandins

Occurrence, nomenclature, Classification, Biogenesis and physiological effects. Synthesis of PGE_2, PGF_2.

Books Suggested

1. Natural Products: Chemistry and Biological Significance, J. Mann, R. S. Davidson, J. B.
2. Hobbs, D. V. Banthrope and J. B. Hatrbnome, Longman, Essex.
3. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
4. Stereo selective Synthesis: A Practical Approach, M. Nogradi, VCH.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettman, M. P. Gupta and A. Marston, Harwood, Academic Publishers.
6. Introduction to Flavonoids, T. A. Geissman.
7. New Trends in Natural Products Chemistry, Atta-ur-Rahman and M. I. Choudhary, Harwood Academic Publisher.
8. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, ELBS.
9. Chemistry of Natural products P. S. Kalsi, Kalyani Publishers.
10. Biosynthesis of steroids, terpenes and acetogenins, J. H. Richards & J. R. Hendrieson.
11. The biosynthesis of secondary metabolites, R. D. Herbert, Chapman & Hall.
12. Chemistry of Organic Natural Products, O. P. Agarwal, Vols. 1 &2, Goel Pubs.
13. Natural Products Chemistry K. B. G. Torsell, John Wiley, 1983.

CHM 404 B - BIO-ORGANIC CHEMISTRY (INTERNAL ELECTIVE)

UNIT-I: Carbohydrates **15 Hrs**

Introduction, Structure and Biological functions of muco polysaccharides, glyco proteins, and Glycolipids. Role of sugars in Biological recognition – Blood Group substances.

UNIT-II: Lipids **15 Hrs**

Introduction – Essential fatty acids – structure and functions of tri glycerol's, Glycerophospholipids, Cholesterol, bile acids prostaglandins – compositions and functioning of lipoproteins.

UNIT-III: Proteins and Nucleic Acids **15 Hrs**

Introduction – classification and properties of proteins and amino acids – structure and conformation, protein synthesis. Synthesis of phenylalanine, Peptide bonds, synthesis of peptides by DCC Method.

Nucleic Acids – Nucleosides – DNA & RNA structure and conformations – replication – translation of genetic material – Gene expression & gene mutation.

UNIT – IV: Enzymes **15 Hrs**

Nomenclature, classification, and properties of enzymes. Factors affecting enzyme catalysis. Enzyme inhibition – reversible and irreversible inhibition. Uses of enzymes in food drink industry, and clinical laboratories.

Books Suggested:

1. A Text-Book of Bio-Chemistry A.V. S Rama Rao.

2. Natural Products Chemistry K. B. G. Torsell, John Wiley 1983.

3. Polymer Chemistry G. S. Mishra.

4. Principles of Bio-Chemistry A.L. Lehniger (worth).

IV Semester Practical Syllabus

405: Estimations of Organic Compounds

I. Estimations

(a) Estimation of Glucose,

(b) Estimation of Phenol,

(c) Estimation of Primary Amine,

(d) Estimation of Ketone by Oxime method.

406: Multistep Synthesis of Organic Compounds

1. Preparations of Benzoic acid from Benzoin,
2. Preparation of benzanilide from benzophenone,
3. Preparation of P – Nitro aniline from Aniline,
4. Preparation of p – Chloro toluene,
5. Preparation of Paracetamol from p-nitro phenol,
6. Preparation of 2,4 – di nitro phenyl hydrazine from Chloro benzene,
7. Preparation of m– Nitro aniline from m – dinitrobenzene.