SHRI GURU RAM RAI UNIVERSITY

(Estd. by Govt. of Uttarakhand, vide Shri Guru Ram Rai University Act no. 03 of 2017)



Syllabus
(M.Sc Chemistry)
Choice Based Credit System(CBCS)

Effective from Academic Session 2018-2019

Patel Nagar, Dehradun, Uttarakhand

Master of Science (CHEMISTRY)-Two Year Programe- Choice Based Credit System

Admission to Master's Program in Chemistry shall be either through entrance examination conducted by University or Merit of qualifying exam and the program shall be based on the choice based credit system in which credit defines the quantum of content/ syllabus prescribed for a course system and determines the number of hours of instruction per week.

The student shall be eligible for admission to a Master's Degree Program in Chemistry after he/she has successfully completed a three year undergraduate degree or earned prescribed number of credits through the examinations conducted by University as equivalent to an undergraduate degree with minimum 45% marks in undergraduate course.

Core courses prescribed for every Semester shall be mandatory for all students registered for the Master's Program in Chemistry and shall carry minimum 86 credits. There shall be Elective courses offered in semester III and IV and shall carry a minimum of 12 credits. A self-study course would comprise of maximum 06 credits of which minimum 03 credits shall be mandatory which shall not be included while calculating grades. The student may choose self-study course either only in one of the two semesters (III/IV).

In order to qualify for a two year master's degree, a student must acquire a minimum of 86 credits including a minimum of 12 credits in electives choosing at least two electives in Semester III and one in Semester IV offered either by the parent department or other departments. The dissertation is a semester long elective course of 09 credits and is mandatory for every student. The dissertation would be allotted in the beginning of III Semester and candidate would submit the thesis/report during IV Semester

The dissertation may be in the form of a minor research work/ project work/ practical training. The students may complete the dissertation work in the department/ other research institutes/ industries, etc. A candidate has to obtain a minimum of 40 % marks in individual paper in university examination as well as in mid term exams and 50% marks in aggregate (Two Sessional Tests marks plus End-Term Examination marks) to pass.

The 2- Year Masters Programme will have the following components:

- 1) Core course: Minimum 74 credits.
- 2) Elective course: Minimum 12 credits
- 3) Dissertation: 09 credits

4) Self study course: Maximum 06 credits (one minimum 03 credits shall be mandatory but not to be included while calculating grades).

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M.Sc. CHEMISTRY SYLLABUS

Course Code	Subjects	L-T-P	Credits	Max Marks
MCHC101	Inorganic Chemistry I	4-0-0	4 .	100
MCHC102	Organic Chemistry I	4-0-0	4	100
MCHC103	Physical Chemistry I	4-0-0	4	100
MCHC104	Spectroscopy and Group theory	4-0-0	4	100
MCHL105	Laboratory Course I	0-0-3	3	100
MCHL106	Laboratory Course II	0-0-3	3	100

Total Core Credits = 22

SEMESTER-II

Course Code	Subjects	L-T-P	Credits	Max Mark
MCHC201	Inorganic Chemistry II	4-0-0	4	100
MCHC202	Organic Chemistry II	4-0-0	4	100
MCHC203	Physical Chemistry II	4-0-0	4	100
MCHC204	Spectroscopy and separation methods	4-0-0	4	100
MCHL205	Laboratory Course I	0-0-3	3	100
MCHL206	Laboratory Course II	0-0-3	2	
10.0	22	0-0-5	2 .	100

Total Core Credits = 22

SEMESTER-III: Select any one discipline of core subjects and any two electives from the list.

Course Code	Subjects	L-T-P	Credits	Max Marks
MCHC301	Organic Synthesis & Photochemistry			
	organic Bynthesis & Photochemistry	4-0-0	4	100
MCHC302	Heterocyclic Chemistry	100		
MCIII 202		4-0-0	4	100
MCHL303	Laboratory Course I	0-0-3		
MCHL304	Yahari	0-0-3	3	100
TCIIL304	Laboratory Course II	0-0-3	-	
		0-0-3	3	100

B: Inorganic Chemistry

Course Code	Subjects			
	Subjects	L-T-P	Credits	Max Marks
MCHC305	Organometallic Chemistry			THAT HAIR
MONGO		4-0-0	4	1.00
MCHC306	Bioinorganic & Supramolecular	100		100
	Chemistry	4-0-0	4	100
MCHL307	Laboratory Course I			100
MCHL308		0-0-3	3	100
CILLS00	Laboratory Course II	0.02	-	
		0-0-3	3	100

Physical Chemistry

Course Code	Subjects	L-T-P	Credits	Max Marks
MCHC309	Chemistry of Materials	4-0-0	4	100
MCHC310	Liquid State	4-0-0	4	
MCHL311	Laboratory Course I	0-0-3	2	100
MCHL312	Laboratory Course II	0-0-3	3	100
		0-0-3	3	100

List of Elective papers (Students have to select any two elective papers)

Course Code	Subjects	L-T-P	Credits	Max Mark
MCHE313	Bioinorganic, Bioorganic & Biophysical			- Mark
	Chemistry	4-0-0	4	100
MCHE314	Organometallic Reagents & Organic	100		
MCHE315	Synthesis	4-0-0	4	100
	Polymers	4-0-0	4	
MCHE316	Photoinorganic Chemistry		4	100
MCHE317	Medicinal Chemistry	4-0-0	4	100
MCHE318		4-0-0	4	100
	Spectroscopy and Solid state chemistry	4-0-0	-	100
t of self study r		7-0-0	4	100

List of self study papers (Students have to select any one par

	Subjects	L-T-P	Credits	Max Marks
MCHS319	Traditional health care system of			Mark Mark
N. Comments	Uttarakhand including ayurvedic medicine		3	100
MCHS320	resticide Chemistry			100
credits=22 (14 core credits + 08 elective credits) and 03 cre		3	100

SEMESTER-IV

A: Organic Chemistry

Course Code MCHC401	Subjects	L-T-P	Credits	Max Marks
MCHL402	Chemistry of Natural Products Laboratory Course I	4-0-0	4	
MCHC403	Dissertation	0-0-3	3	100
Inorganic Ch	emistry		9	300

Course Code		Subjects			
	N		L-T-P	Credits	Max Marks
	At-				max marks

MCHC404	Inorganic Polymers	4-0-0	4	100
MCHL405	Laboratory Course I	0-0-3	3	100
MCHC403	Dissertation		9	300

C: Physical Chemistry

Course Code	Subjects	L-T-P	Credits	Max Marks
MCHC406	Advanced Quantum Chemistry	4-0-0	. 4	100
MCHL407	Laboratory Course 1	0-0-3	3	100
MCHL403	Dissertation		9	300

List of Elective papers (Students have to select any one elective papers)

(Course Code	Subjects	L-T-P	C 111	
		r-1-L	Credits	Max Marks
MCHE408	Green Chemistry	100		
		4-0-0	4	100
MCHE409	Modern Techniques of Chemical analysis	400	-	
Memmu		4-0-0	4	100
MCHE410	Computers and Biostatistics	4-0-0	1	
MCHE411	Paul 101	4-0-0	4	100
MCHE411	Environmental Chemistry	4-0-0	1	100
MCHE412	Chamiatau of		4	100
	Chemistry of macromolecules	4-0-0	4	100
				100

List of self study papers (Students have to select any one paper)

Course Code	Cubing one paper)			
	Subjects	L-T-P	Credits	Max Marks
MCHS413	Analytical Chemistry		3	
MCHS414	Titrimetric Analysis			100
tal credits=20 (16 care credits + 0.4 d.)			3	100

Total credits=20 (16 core credits + 04 elective credits) and 03 credits of self study

Journal club will include the reading, presentation and to develop writing skills in view of thesis

The develop writing skills in view of thesis.

The develop writing skills in view of thesis.

The thesis evaluation will be of 180 marks and 60 marks for academic performance and 60 for presentation/viva.

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Semester- I

MCHC101: Inorganic Chemistry I

M.M: 100

Credit:4 (Four Lectures Per Week)

Stercochemistry and Bonding in Main Group Compounds

VSEPR model and its shortcomings. Hybridization and three-center bonds. Bents rule and energetics of hybridization. Walsh's diagrams for tri and tetraatomic molecules. $p\pi$ - $p\pi$ and $p\pi$ - $d\pi$ bonding.

Metal-Ligand Equilibria in Solution

Thermodynamic and kinetic stability of complexes. Stepwise and overall formation constants and their interaction. Trends in K value. Irving-Willams series. Chelate effect and its thermodynamic origin. Factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand.

Reaction Mechanism of Transition Metal Complexes

Energy profile of a reaction and reactivity of metal complexes. Inert and labile complexes. Ligand substitution reactions in octahedral complexes i.e. SN1,SN2 and SN1CB mechanism. Anation reactions without metal ligand bond cleavage, Electron transfer reactions(Redox reactions). Outer and inner sphere mechanism (OSM and ISM).Reactions of coordinated ligands. Substitution reactions in square-planer complexes.

Theories of Coordination Compounds

Crystal field theory, factors affecting the magnitude of 0. Consequences of crystal field splitting. merits and limitations of CFT Jahn-Teller distortion and its consequences on complex formation. Evidence of covalent character in Metal-Ligand bonding. Molecular orbital theory as applied to octahedral, tetrahedral and square

Books suggested

Advanced Inorganic Chemistry Vth Ed., F.A. Cotton and G. Wilkinson, John Wiley, (1988).

Advanced Inorganic Chemistry VIth Ed., F.A. Cotton, G Wilkinson, C.A. Murillo and M. Bochmann, John

Inorganic Chemistry, J.E.House, Academic Press, (2008) Inorganic chemistry, A Unified Approach, IInd Ed., W W. Porterfield, Academic Press, (1993). Coordination Chemistry, IIIrd Ed., D Banerjea, Asian Book Pt. ltd., (2009)

Coordination Chemistry, Jihrd Ed., D Banerjea, Asian Book Pt. Itd., (2009)

Inorganic Chemistry, 3th Ed., G L Miessler and D.A. Tarr, Pearson Education, Inc. (2004)

Concise Inorganic Chemistry, J.D. Lee, 5th Ed., Chapman & Hall (1996).

Inorganic Chemistry, 3th Ed., Shriver & AtkinsOxford (1999).

Inorganic Chemistry, 3th Ed., Alan G. Sharpe, Addison-Wesley (1992).

Inorganic Chemistry, 4th Ed., J.E. Huheey, Harper & Row (2000).

Chemistry of the Elements, 2th Ed., N.N. Greenwood and A. Earnshaw, Butterworth. Heinemann (1997). 12 Inorganic Electronic Spectroscopy, 2nd Ed., A.B.P. Lever, Elsevier (1986).

13 Magnetochemistry, R.L. Carlin, Springer Verlag (1986).

MCHC102: Organic Chemistry I

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Nature of Bonding in Organic Molecules

Hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non benzenoid compounds, alternant and non alternant hydrocarbons. Huckel's rule, energy level of π-molecular orbitals, annulenes, antiaromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent, crown ether complexes and cryptands, inclusion compounds, cyclodextrin, catenanes and rotaxanes.

Unit II

Stereochemistry

Conformational analysis of cycloalkane, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis, chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit III

Reaction Mechanism: Structure and Reactivity

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Effect of structure on reactivity - resonance and field effects, steric effect, quantitative treatments. Hammett equation and linear free energy relationship, Substituent and reaction constants, Tast equation. Methods of determining Reaction mechanism

Unit IV

Aliphatic Nucleophilic Substitution

SN1, SN2 and mixed SN1 and SN2 mechanism. The neighbouring group mechanism, neighbouring group participation (by π - and σ bonds). Anchimeric assistance. SN1 mechanism- Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophilic group, leaving group and reaction medium, ambident nucleophile.

Unit V

Aliphatic Electrophilic Substitution

Bimolecular mechanism- SE2. The SE1 mechanism, electrophilic substitution accompanied by double bond shift. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Books suggested:-

Advanced Organic Chemistry, Reaction, Mechanism and Structure, Jerry March, 6th Ed., John Wiley.

Advanced Organic Chemistry, Carey and Sundberg, Springer Verlag, Germany.

- 3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes.
- 4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press. 5. Organic Chemistry, Boyd and Morrison, Prentice Hall of India.

- 6. Modern Organic Reactions, H.O. House, Benjamin.
- 7. Principles of Organic Synthesis, Norman and Coxon, Blackwell.
- 8. Reaction Mechanism in Organic Chemistry, Mukherji and Singh, Macmillan. 9. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
- 10. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

MCHC103: Physical Chemistry I

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Quantum Chemistry: Basic Principles Of Quantum Mechanics

Operators, Eigen values and Eigen functions, Normalisation, Hiensenberg Uncertainity Principle, de Broglie equation, Angular Momentum, Ladder operators . Hermitian adjoint.

Unit II

Quantum Chemistry: Introduction to Exact Quantum Mechanical Results

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Unit III

Quantum Chemistry: Approximate Methods

The variation theorem, linear variation principle, perturbation theory (first order and nondegenerate).

Unit IV

Quantum Chemistry: Chemical Bonding In Diatomics

Elementary Concepts of Molecular Orbital and Valence Bond Theory, Huckel Molecular Orbital Theory for conjugated []-electron systems.

Thermodynamics: Classical Thermodynamics

Brief resume of concepts of laws thermodynamics, free energy, chemical potential and entropies. Partial molar properties: partial molar free energy, partial molar volume and partial molar heat content and their significance. Determination of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient. Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength

Unit VI

Surface Chemistry: Adsorption

Surface tension, capillary actions, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon), catalytic activity at surfaces.

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. Coulson's Valence, R. McWeeny, ELBS,

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MCHC104: Spectroscopy and Group theory

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Unifying Principles

Electromagnetic radiation, interacton of electromagnetic radiation with matter. Absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment, selection rules, intensity of special lines, Born-oppenheimer approximation, rotational, and electronic energy levels

Unit II

Atomic Electronic Spectroscopy

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

Unit III

Ultra Violet and Visible Spectroscopy

Electronic transitions (185-800 nm), Beer- Lambert Law, Effect of solvent on electronic transitions, Ultra Violet bands of carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Steric effect in biphenyls, Fieser- Woodward rules for conjugated dienes and carbonyl compounds, ultra violet spectra of aromatic and heterocyclic compounds.. Applications of UV- visible spectroscopy in organic chemistry.

Unit IV

Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, Zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, virbration-rotation spectroscopy; affecting the band positions and intensities, far IR region., metal-ligand vibrations,

.Unit V

Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroups, conjugacy relation and classes. Point symmetry group, Schonflies symbols, explicitly).

Books Suggested:

1. Modern Spectroscopy, J.M. Hollas, John Wiley.

2. Physical Methods for Chemistry, R.S. Drago, Saunders Company.

3. Chemical Applications of Group Theory, F.A. Cotton.

4. Introduction of Molecular Spectroscopy, G.M. Barrow, McGraw Hill.

5. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.

6. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, New Age International.

MCHL105: Laboratory Course I

M.M:100

Credit:3(Nine hrs per week)

Part 1: Inorganic Chemistry

Qualitative analysis of mixtures by semi-micro methods containing not more than six cations and arrions

- Rare-earth elements
- (ii). Anions, which have not been done in under graduate practicals.
- (iii). Insolubles.

Part 2: Organic Chemistry

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (solid-solid or liquid and solid) using TLC and Paper Chromatography, Chemical tests and spectroscopic analysis.

Part 3: Physical Chemistry

Chemical Kinetics

- 1. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic
- 2. Determination of the velocity constant of hydrolysis of an ester.
- 3. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the
- 4. Flowing clock reactions (Ref: Experiments in Physical Chemistry by Showmaker).
- 5. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted

MCHL106: Laboratory Course II

M.M:100

Credit:3(Nine hrs per week)

Part 1: Inorganic Chemistry Chromatography Separation of cations and anions by-Paper Chromatography Thin Layer Chromatography Ion Exchange Chromatography

Part 2: Organic Chemistry Organic Synthesis Acetylation: Acetylation

Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol. Grignard reaction: Synthesis of triphenylmethanol from benzoic acid.

Sandmeyer reaction: p-Chlorotoluene from p-toluene

Part 3: Physical Chemistry

Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.

Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO4, BaSO4) conductometrically.

3. Determination of the strength of strong and weak acids in a given mixture conductometrically.

4. To study the effect of solvent on the conductance of AgNO3/CH3COOH and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixture's (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.

5. Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using

Debye Huckel's limiting law.

Semester-II

MCHC201: Inorganic Chemistry II

Credit:4 (Four Lectures Per Week)

M.M: 100

Electronic Spectra & Magnetic Properties of Transition Metal Complexes.

Types of absorption spectra. Spectral terms. Russell-Saunders states. Selection rules for electronic transitions in complexes. Width of absorption spectral bands, Terms generated in ligand fields. Orgel and Tanabe-Sugano correlation diagrams for d1 to d9 states. Racah parameters. Charge transfer spectra. Magnetic moments, magnetic exchange coupling and spin crossover.

Metal-π-Complexes and organometallic Compounds.

Metal carbonyl complexes. Preparation, properties and uses. Nature of bonding in metal carbonyls and carbon monoxide analogs i.e. nitrosyls and dinitrogen complexes. Evidence for back bonding in complexes. Nature of M-C bond Synthesis, bonding and uses of organometallic compounds, two electron ligands (olefinic and acetylenic complexes), three electron ligands (allylic complexes), four electron ligand (butadiene and cyclobutadiene complexes), five electron ligand (ferrocene complexes).

Unit III

Metal Clusters

Polyhedral boranes and borane anions. Synthesis, reactivity, bonding and topology of boranes.: Wade's rules. Carboranes, metalloboranes and metallocarboranes. Metal carbonyls and halides as clusters. Metal carbonyl

Unit IV

Silicates

Principles of silicates. Structure and classification of silicates. Asbestos, Zeolites and Ultramarines as silicate

Books suggested

Advanced Inorganic Chemistry Vth Ed., F.A. Cotton and G. Wilkinson, John Wiley, (1988).

Advanced Inorganic Chemistry VIth Ed., F.A. Cotton, G Wilkinson, C.A. Murillo and M. Bochmann,

Inorganic Chemistry, J.E.House. Academic Press, (2008)

4. Inorganic chemistry, A Unities Apparach, IInd Ed., W W. Porterfield, Academic Press, (1993). 5. Coordination Chemistry, Illrd Ed., D Banerjea, Asian Book Pt. ltd., (2009)

5. Coordination Chemistry, Illrd Ed., D Banerjea, Asian Book Pt. Itd., (2009)
6. Inorganic Chemistry, 3 Ed., G.L. Miessler and D.A. Tarr, Pearson Education, Inc. (2004)
7. Concise Inorganic Chemistry, J.D. Lee, 5th Ed., Chapman & Hall (1996).
8. Inorganic Chemistry, 3th Ed., Shriver & Atkins, Oxford (1999).
9. Inorganic Chemistry, 4th Ed., J.E. Huheey, Addison-Wesley (1992).
10. Inorganic Chemistry, 4th Ed., J.E. Huheey, Harper & Row (2000).
11. Chemistry of the Elements, 2th Ed., N.N. Greenwood and A. Earnshaw, Butterworth. Heinemann (1997).
12. Inorganic Electronic Spectros.
13. Magnetochemistry, R.L. Carl.
14. A.B.P. Lever, Elsevier (1986). 13. Magnetochemistry, tel. Chemistry Eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty,

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MCHC 202: Organic Chemistry II

M.M: 100

Credit:4 (Four Lectures Per Week)

Aromatic Electrophilic Substitution

Orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrate and electrophiles. Diazonium coupling, Vilsmeir Haak reaction, Gattermann-Koch reaction.

Unit II

Aromatic Nuccleophilic Substitution

The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity- effect of substrate structure, leaving group and attacking nucleopile. The von Rictor, Sommelet-Hauser, and Smiles rearrangements.

Unit III

Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism of an aromatic substrate, neighboring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Unit IV

Addition to Carbon-Carbon Multiple Bonds

Mechanism and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to eye lopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric

Unit V

Addition to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Wittig reaction. Mechanism of condensation reactions involving enolates- Knoevenagel, Claisen, Mannich Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Unit VI

Elimination Reactions

The E2, E1 and E1cB mechanisms and their stereochemistry. Orientation of the double bond. Reactivity- effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and

Unit VII

Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann. Correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and suprafacial additions, 4n, and 4n+2 systems. Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1, 3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements- suprafacial and antarafacial shiffs of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements. Claisen, Cope and aza- Cope

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Books suggested:-

- 1. Advanced Organic Chemistry- Reaction, Mechanism and Structure, Jerry March, John Wiley.
- 2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
- 3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- 4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
- 5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
- 6. Modern Organic Reactions, H.O. House, Benjamin.
- 7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackwell,
- 8. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
- 9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
- 10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
- 11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

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MCHC203: Physical Chemistry II

M.M: 100

Credit:4 (Four Lectures Per Week)

UnitI

Chemical Dynamics

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory. Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogenbromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction), homogeneous catalysis, kinetics of enzymes reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

Unit II

Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws- (using Lagrange's method of undetermined multipliers). Partition functions- translational, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partition functions. Applications of partition functions. Heat capacity behaviour of solids- chemical equilibria and chemical equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics - distribution law and application to helium.

Unit III

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, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

UnitIV

Electrochemistry

Electrochemistry of solutions, Debye-Huckel, Onsager treatment and its extension, ion solvent interactions. Thermodynamics of electrified interface equations. Structure of electrified interfaces. Guoy Chapman. Stern. Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Electrocatalyis - influence of various parameters. Hydrogen electrode. Bioektrochemistry, threshold membrane phenomena. Polarography theory, Ilkovic equation, half wave potential and its significance. Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and

Books suggested:-

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

2. Coulson's Valence, R. McWeeny, ELBS.

 Coulson's Valence, R. I.
 Modern Electrochemistry, Vol. I & II, J.O.M. Bockris and A.K.N. Reddy, Plenum. 4. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.

Quantum Chemistry, Ira N. Levine, Prentice Hall.

MCHC204: Spectroscopy and Separation methods

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Molecular Electronic Spectroscopy

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of excited states, Franck-Condon principle, Dissociation and pre-dissociation, electronic spectra of polyatomic molecules. Emission spectra, radiative and non-radiative decay, internal conversion,

Unit II

Magnetic Resonance Spectroscopy

Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factor influencing chemical shift, deshielding, spin-spin interaction, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A2B2 etc.), spin decoupling, basic ideas about instrument, NMR studies of nuclei other than proton-13C, 19F. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

Unit III

Mass Spectrometry

Introduction, ion production-El, Cl, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, Molecular ion peak, Meta-stable peak, McLafferty rearrangement. Nitrogen Rule, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Introduction to negative ion Mass

Unit IV

Chromatographic Methods

Principle, instrumentation and applications of gas liquid chromatography and HPLC. Ion exchange chromatography: cationic and anionic exchanges and their applications. Van-Deemter equation (no derivation), concept about HEPT-plate theory and rate theory. Applications.

Unit V

Radio Analytical Methods

Basic principles and types of measuring instruments, isotope dilution techniques: principle of operations and uses.

Books Suggested:

- 1. Modern Spectroscopy, J.M. Hollas, John Wiley.
- 2. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood. 3. Physical Method for Chemistry, R.S. Drago, Saunders Company.
- 4. Introduction of Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
- 5. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
- 6. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford. 7. Introduction to Magnetic Resonance, A. Carrington, A.D. Maclachalan, Harper & Row. 8. High Performance Liquid Chromatography, Heinz Engelhardt.
- 9. Instrumental Methods of Chemical Analysis, Willard, Meritt, Dean & Settle (Wiley Eastern).

MCHL205: Laboratory Course I

M.M:100

Credits:3(Nine hrs per week)

Part 1: Inorganic Chemistry

Quantitative Analysis of mixtures of two metal ions involving Volumetric (by complexometric titration using masking and demasking agents) and gravimetric analysis.

Part 2: Organic Chemistry

Synthesis of Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation. Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate Aromatic electrophilic Substitutions: Synthesis of pnitroaniline and p-bromoaniline. The products may be characterized by Spectral Techniques where possible.

Part 3: Physical Chemistry Solutions

- 1. Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
- Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

MCHL206: Laboratory Course II

M.M:100

Credits:3(Nine hrs per week)

Part I: Inorganic Chemistry

Preparations

Preparation of selected inorganic compounds:

VO (acac)2

TiO (C9H8NO)2. 2H2O

cis-K[Cr(C2O4)2 (H2O)2]

Na[Cr(NH3)2(SCN)4]

Mn (acac)3

K3 [Fe (C2O4)3] 3H2O

Prussian Blue, Turnbull's Blue

Co [(NH3)6] Cl3

[Cu (en)2 (H2O)2] 12

Cu2Hgl4

[Co (Py)2C12]

[Ni (NH3)6] Cl2

Tris-(thiourea) copper (I) sulphate [Cu (tu)3] SO4.2H2O

K3[Cr (C2O4)3]

Part 2: Organic Chemistry

Quantitative Analysis

- 1. Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation
- 2. Estimation of amines/phenols using bromate bromide solution/or acetylation method.
- 3. Determination of Iodine and Saponification values of an oil sample
- 4. Determination of DO, COD and BOD of water sample.

Part 3: Physical Chemistry

Potentiometry/pH-metry

- Determination of strengths of halides in a mixtures potentiometrically.
- Determination of the valency of mercurous ions potentiometrically.
- Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter. Determination of temperature dependence of EMF of a cell. 4.
- Determination of the formation constant of silver-ammonia complex and stiochiometry of the complex
- Acid-base titration in a non-aqueous media using a pH meter.
- Determination of activity and activity coefficient of electrolytes.
- Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating
- Determination of the dissociation constant of monobasic/dibasic by Albert-Serjeant method.
- 10. Determination of thermodynamic constants ΔG , ΔS and ΔH for the reaction by e.m.f. method.

ZnSO4 + 2H

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Semester- III

MCHC301: Organic Synthesis and Photochemistry

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Disconnection Approach

An introduction to synthons and synthetic equivalents disconnection approach, functional group interconversions, the importance of order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions and amine synthesis.

Unit II

Protecting Groups

Principle of protection of alcohols, amine, carbonyl and carboxyl groups

One Group and Two Group C-C Disconnections

Alcohols and carbonyl compounds regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis. Diels-Alder reaction, 1,3-difunctional compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensations. Micheal addition and Robinson annelation.

Unit IV

Determination of Reaction Mechanism

Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions, photodissociation, gas-phase photolysis.

Unit V

Photochemical Reactions

Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4and 1,5-dienes. Intramolecular reactions of carbonyl compounds-saturated cyclic and acyclic, β,γ-unsaturated and a,β-unsaturated compounds. Cyclohexadienones. Intramolecular cycloaddition reactions-dimerisation and oxetane formation. Isomerisation, additions and substitutions.. Photo-Fries rearrangement, Barton reaction.

Books Suggested:

Modern Synthetic Reactions, H.O. House, W.A. Benjamin.

Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.

Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.

Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional. Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press.

Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.

Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, New Age International

Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication Molecular Photochemistry, N.J. Turro, W.A. Benjamin

Introductory Photochemistry, A. Cox and T. Camp, McGraw Hill-

Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson

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MCHC302: Heterocyclic Chemistry

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Nomenclature of Heterocycles

Replacement and Systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles

Unit II

Aromatic and Non-aromatic Heterocycles

General chemical behaviour of aromatic heterocycles, classification (structural type), Heteroaromatic reactivity and tautomerism in aromatic heterocycles Strain -bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interactions. Stereoelectronic effects, aromatic and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic, electrophilic interactions.

Unit III

Small Ring Heterocycles

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes

Unit IV

Benzo-Fused Five-Membered Heterocycles

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

Six-Membered Heterocycles with One, Two or More Heteroatoms

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridines Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones Synthesis and reactions of diazines, triazines, tetrazines and thiazines

Unit VI

Seven-and Large-Membered Heterocycles

Synthesis and reactions of azepines, oxepines, thiepines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines

Books Suggested:

Heterocyclic Chemistry Vol. 1 & 2, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag

The Chemistry of Heterocycles, T. Eigher and S. Hauptmann, Thieme.

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

Heterocyclic Chemistry, T.L. Gilchrist, Longman Scietific Technical

5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science. An introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley

- Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon
- Natural Products: Chemistry and Biological Significance, J.Mann, R.S. Davidson, J.B. Hobbs, D.V.

). Organic Chemistry, Vol 2, I.L. Finar, ELBS.

0. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH

MCHL303: Laboratory Course I

M.M:100

Credits:3(Nine hrs per week)

Qualitative Analysis

Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid), using TLC for checking the purity of the separated compounds. Preparation of derivatives and spectral analysis.

Books Suggested

- 1. Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman and GS Kriz, Saunders College Publishing, Philadelphia, New York.
- Operational Organic Chemistry, A Laboratory Course, Second Edition, JW Lehman, Allyn & Bacon, Inc.
- Microscale Organic Experiments KL Willianson, DC Health & Co. Le Xington.
- Laboratory Manual of Organic Chemistry, RK Bansal, New Age International, Delhi.

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MCHL304: Laboratory Course II

M.M:100

Credits:3(Nine hrs per week)

Multi-step Synthesis of Organic Compounds

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

Photochemical reaction

Benzophenone → Benzpinacol → Benzpinacolone

Beckmann rearrangement: Benzanilide from benzene

Benzene → Benzophenone → Benzophenone oxime → Benzanilide

Benzilic acid rearrangement: Benzilic acid from benzoin

Benzili → Benzilic acid

Synthesis of heterocyclic compounds

Skraup synthesis: Preparation of quinoline from aniline. Fisher-Indole synthesis: Preparation of 2-phenyl indole from phenylhydrazine.

Experiments related to elective papers.

Books Suggested

- 1. Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman and GS Kriz,
- 2. Operational Organic Chemistry, A Laboratory Course, Second Edition, JW Lehman, Allyn & Bacon, Inc.
- 3. Microscale Organic Experiments KL Willianson, DC Health & Co. Le Xington.
- 4. Laboratory Manual of Organic Chemistry, RK Bansal, New Age International, Delhi.

MCHC305:Organomettalic Chemistry

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Alkyls and Aryls of Transition Metals Alkyls and aryls of transition metals, nature of metal carbon bond, routes of synthesis, stability and decomposition pathways and their structure. Alkyls and aryls of s-block and p-block elements. Comparison of such transition and non-transition element derivatives. Organocopper in organic synthesis.

Unit II

Compounds of Transition metal-carbon multiple bonds Alkylidenes, alkylydines, low valent carbones and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the figands, role in organic synthesis.

Unit III

Transition Metal π-Complexes Transition Metal π-Complexes with unsaturated organic molecules. Alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes; preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Unit IV

Metal Compounds with bonds to Hydrogen

Unit V

Transition metal compounds with bonds to hydrogen

Homogeneous Catalysis Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reaction, activation of C-H bond.

UnitVI

Fluxional Organometallic Compounds Fluxionality and dynamic equilibria in compounds such as $\eta 2$ -olefin, $\eta 3$ -

Books Suggested:

- 1. Principle and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.P. Norton and R.G. Finke. University Science Books. 2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley.
- 3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
- 4. Organometallic Chemistry, R.C. Mehrotra and A. Singh; New Age International. 5. Organometallic Compounds, NLH Green, Chapman & Hall, U.K.
- 6. Principles of Organometallic Chemistry, G.E. Coates, MLH Green, P. Powell, Chapman & Hall, U.K.

MCHC306: Bioinorganic and Supramolecular Chemistry

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Metal Storage Transport and Biomineralization Ferritin, Transferrin, and siderophores

Calcium in Biology Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins.

Metalloenzymes Zinc enzymes-carboxypeptidase and carbonic anhydrase. Iron enzymes-catalase, peroxidase and cytechrome P-450. Copper enzymes-superoxide dismutase. Molybdenum oxatransferase enzymesxanthine oxidase. Coenzymes vitamin B12.

Unit IV

Metal-Nucleic Acid Interactions Metal ions and metal complex interactions. Metal complexes-nucleic acids.

Unit V

Metals in Medicine Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and

Unit VI

Supramolecular Chemistry Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co-receptor molecules and multiple recognition. H-bonds in supramolecular structures. Use of H-bond in crystal engineering and molecular recognition. Chelate and macrocyclic effects. Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules. Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices, supramolecular photochemistry, supramolecular electronic, ionic and switching devices. Some examples

Books Suggested:

- 1. Supramolecular Chemistry, J.M. Lehn, VCH.
- 2. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 3. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books. 5. Progress in inorganic Chemistry, vols 18 and 38 ed. J.J. Lippard, Wiley.

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MCHL307: Laboratory Course I

M.M:100

Credits:3(Nine hrs per week)

Preparation Synthesis of selected inorganic compounds/complexes and their characterization by IR, electronic spectra (UV & Visible), NMR, Mossbauer, ESR and magnetic susceptibility etc. measurement. Selection can be made from the following or any other from the existing literature.

- Cis and Trans isomers of [Co(en)2Cl2] Cl. J. Chem. Soc., 1960, 4369.
- Metal acetylacetonates: Cr(acac)3; Vanadyl acetylacetonate, Cu(acac)2. H2O etc. Inog. Synth., 1957, 5, 130; 1, 183.
- Ferrocene J. Chem. Edu., 1966, 43, 73; 1976, 53, 730.
- Cr(III) complexes: [Cr(H2O)6](NO3)3.3H2O;[Cr(H2O)4 Cl2] Cl.2H2O; [Cr(en)3]Cl3 Inorg. Synth., 1972, 13, 184.
- Tin (IV) iodide, Tin (IV) chloride, Tin (II) iodide. Inorg. Synth., 1953, 4, 119.
- · Mixed valence dinuclear complexes of manganese (III, IV).
- · Preparation of triphenyl phosphine and its transition metal complexes.
- Reaction of Cr (III) with multidentate ligand, a kinetic experiment (visible spectra of Cr-EDTA complex). J. Am. Chem. Soc., 1953, 75, 5670.
- Other new synthesis reported in literature.
- Bromination of Cr (acac)3. J. Chem. Edu., 1986, 63, 90.
- Preparation of copper glycine complex-cis and trans bis glycinato copper (II). J. Chem. Edu., 1982, 59,
- Relative stability of Tin (IV) and Pb (IV), Preparation of ammonium hexachlorostannate,(NH4)2SnCl6 and ammonium hexachloroplumbate; (NH4)2 PbCl6.

Books Suggested

- 1. Vogel's Text Book of Qualitative Analysis, ELBS.
- 2. Vogel's Text Book of Quantitative Analysis, ELBS.
- 3. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.

MCHL308: Laboratory Course II

M.M:100

Credits:3(Nine hrs per week)

Analysis of ores, alloys and inorganic substances by various chemical methods.

Books Suggested

- L Vogel's Text Book of Qualitative Analysis, ELBS .
- 2. Vogel's Text Book of Quantitative Analysis, ELBS.
- 3. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.

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MCHC309: Chemistry of Materials

M.M: 100

Credit:4 (Four Lectures Per Week)

Multiphase Materials Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications

Glasses, Ceramics, Composites and Nanomaterials Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications. Microscopic composites; dispersion-strengthened and particle-reinforced, firbe-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.

Unit III

Thin Films and Langmuir-Blodgett Films Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuiur-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

Unit IV

Liquid Crystals Mesomorphic ehavior, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic-nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

Unit V

Polymeric Materials Molecular shape, structure and configuration, crystallinity, stress-strain ehavior, thermal ehavior, polymer types and their applications, conducting and ferro-electric polymers.

Unit VI

Ionic Conductors Types of ionic conductors, mechanism of ionic conductors, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

Unit VII

High Te Materials Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high Tc materials, applications of high Tc

Books Suggested

- Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
- 2. Material Science and Engineering, An Introduction, W.D. Callister, Wiley.
- Principles of the Solid State, H.V. Keer, Wiley Eastern.
- 4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS. 5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
- 5. Handbook of Liquid Crystals, Kelker and Hatz, Chemie Verlag.
- 7. Inorganic Materials:Recent Advances,Editors D.Bahadur et al.,Narosa
- 3. Ion Conducting Materials: Theory and Applications, Editor A. R. Kulkarni, Narosa.

MCHC310: Liquid State

M.M: 100

Credit:4 (Four Lectures Per Week)

General Properties of Liquids (a) Liquids as dense gases, liquids as disordered solids, some thermodynamics relations, internal pressure and its significance in liquids. Equations of state, critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids. Additivity of pair potential approximation.

(b) A classical partition function for liquid for liquids, correspondence principle, configuration integral, configuration properties.

Unit II

Theory of Liquids Theory of liquids, partition function method or model approach, single cell models, communal energy and entropy, LTD model, significant structure model.

Unit III

Distribution Function and Related Equations Radial distribution function method, equation of state in terms of RDF. Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.

UnitIV

Methods for Structure Determination and Computational Techniques Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy. Computation Techniques- Monte Carlo and molecular dynamics methods.

Supercooled and Ionic Liquids. Supercooled and ionic liquids, theories of transport properties; non Arrhenius ehavior of transport properties, Cohen-Turnbull free volume model, configurational entropy model, Macedo-Lltovitz hybrid model, glass transition in supercooled liquids.

Books Suggested

- I. An Introduction to Liquid State, P.A. Egeistaff, Academic Press.
- 2. The Dynamic Liquid State, A.F.M. Barton, Longman.
- 3. Introduction to Statistical Thermodynamics, T.L. Hill, Addison Wiley.
- 4. The Liquid State, J.A. Pryde.
- 5. Significant Liquid Structures, H. Eyring and M.S. John.

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MCHL311: Laboratory Course I

M.M:100

Credits:3(Nine hrs per week)

- · Verification of the law of photochemical equivalence.
- · Order of reaction by:
 - (a). Isolation Method.
 - (b). Half life period method
 - (c). Integration method
- Temperature coefficient of a reaction.
- · Energy of activation of a reaction.
- · Entropy of a reaction
- · Determination of pH by following methods:
 - (a). Electrical Conductivity.
 - (b). E.M.F.
 - (c). Polarography

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MCHL312: Laboratory Course II

M.M:100

Credits:3(Nine hrs per week)

- Hydrolysis of the salts by following methods:
 - (a). Cryoscopic
 - (b). Electrical Conductivity.
 - (c). E.M.F.
- Study of complex formation by the following methods and determination of stability constant wherever
 - (a). Cryoscopic
 - (b). Electrical Methods.
 - (c). E.M.F.
- Determination of solubility of sparingly soluble salts by the following methods:
 - (a). Electrical Conductivity.
 - (b). E.M.F.
- Dissociation constants of polybasic acids.

LIST OF ELECTIVE PAPERS IN IIIrd SEMESTER

MCHE313: Bioinorganic, Bioorganic & Biophysical Chemistry

Credit:4 (Four Lectures Per Week)

M.M: 100

Unitl

Bioinorganic Chemistry

Metal Ions in Biological Systems, Na+/K+ Pump

Essential and trace metals. Role of metal ions in biological processes. Na*/K* Pump.

Bioenergetics and ATP Cycles

DNA polymerization, glucose storage, metal complexes in transmission of energy; chlorophylls, photo system I and photo system II in cleavage of water. Model systems.

Transport and Storage of Dioxygen

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

Unit II

Bioorganic Chemistry

Enzymes & Mechanism of Enzyme Action

Introduction and historical perspective, chemical and biological catalysis, properties of enzymes-catalytic power, specificity and regulation. Fischer's lock and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed, mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition. Transitionstate theory, acid-base catalysis, covalent catalysis, strain of distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Kinds of Reactions Catalysed by Enzymes

Nucleophillic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, -cleavage and condensation, some isomerization and rearrangement reactions. Enzyme

Biophysical Chemistry

Biological Cell and its Constituents, Cell Membrane and Transport of Ions

Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil

Standard free energy change in biological reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP

Suggested
Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books. 2. 3.

Principles of Bioinorgame Chemistry, S.J. Elppard and J.W. Berg, University Science Books.

Bioinorganic Chemistry, I. Berteni, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.

Bioinorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny,

- 5. Enzyme Chemistry: Impact and Applications, Ed. Collins J Sucking, Chapman and Hall.
- 6. Enzymes Mechanism Ed, M.I. Page and A. Williams, Royal Society of Chemistry.
- 7. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.
- 8. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
- 9. Enzymatic Reaction Mechanism, C. Walsh, W.H. Freeman.
- 10. Enzymatic Structure and Mechanism, W.H. Freeman.
- 11. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
- 12. Biochemistry, L. Stryer, W.H. Freeman.
- 13. Biochemisty, J. David Rawn, Neil Patterson.
- 14. Biochemistry, Voet and Voet, John Wiley.
- 15. Outlines of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley.

MCHE314: Organometallic Reagents & Organic Synthesis

Credit:4 (Four Lectures Per Week)

M.M: 100

Principles, preparations, properties and applications of the following in organic synthesis with mechanistic details

Group I and II metal organic compounds

Li and Hg compounds.

Transition metals

Pd, Ni and Cr compounds.

Other elements

Si and B compounds.

UnitII

Introduction. Different oxidative processes. Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and inactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and tha Ilium (III) nitrate.

UnitIII

Reduction

Introduction. Different reductive processes. Reduction of hydrocarbons- alkenes, alkynes and aromatic rings. Reduction of carbonyl compounds (aldehydes, ketones, acids and their derivatives). Epoxides. Reduction of nitro, nitroso, azo and oxime groups. Hydrogenolysis.

Unit IV

Rearrangements

General mechanistic considerations-nature of migration, migratory aptitude, memory effects A detailed study of the following rearrangements Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction

UnitV

Metallocenes, Nonbenzenoid Aromatics and Polycyclic Aromatic Compounds General considerations, synthesis and reactions of some representative compounds

Books Suggested:

Modern Synthetic Reactions, H.O. House, W.A. Benjamin.

Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March. 6th Edn., John Wiley. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.

Advanced Organic Chemistry Part B, F.A. Carey and R.J. Sundberg, Plenum Press. 6. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.

7. Designing Organic Synthesis, S. Warren, Wiley.

8. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlag VCH.

MCHE315: Polymers

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain, ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization n homogenous and heterogeneous systems.

Unit II

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testingtensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion

Unit III

Structure and Properties Morphology and order in crystalline polymers, configurations of polymer chains. Crystal structure of polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties, crystallinemelting point Tm, melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg. Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property

Unit IV

Plastic, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and

Books Suggested

- 1. Textbook of Polymer Science, F.W. Billmeyer Jr, Wiley.
- 2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
- 3. Functional Monomers and Polymers, K. Takemoto, Y. inaki and R.M. Ottanbrite. 4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
- 5. Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional.

MCHE316: PhotoInorganic Chemistry

M.M: 100

Credit:4 (Four Lectures Per Week)

Basics of photochemistry Absorption, excitation, photochemical laws, electronically excited states-life times, measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and nonradiative process, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes.

Unit II

Properties of Excited States Structure, dipole moment, acid-base strengths, reactivity. Photochemical kineticscalculation of rates of radiative processes. Biomolecular deactivation-quenching.

Unit III

Excited States of Metal Complexes Excited states of metal complexes: Comparison with organic compounds. electronically excited states of metal complexes. Charge-transfer spectra, charge transfer excitations, methods for obtaining chargetransfer spectra.

Unit IV

Ligand Field Photochemistry Photosubstitution, photo oxidation and photo reduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

Unit V

Redox Reactions by Excited Metal Complexes Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenanthroline complexes), illustration of reducing and oxidizing character of Ruthenium2+, (bipyridyl complex, comparison with Fe (bipy)3); role of spin-orbit coupling, life time of these complexes. Application of redox processes of electronically excited states for catalytic purpose, transformation of low energy reactants into high-energy products, chemical energy into light.

Unit VI

Metal Complex Sensitizers Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction

Books Suggested:

- 1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
- 2. Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
- 3 Progress in Inorganic Chemistry, vol. 30, ed. S.J. Lippard, Wiley.
- 4. Co-ordination Chem. Revs., 1975, 15, 321; 1981, vol. 39, 121, 131; 1990, 97, 313
- 5. Photochemistry of Co-ordination Compounds, V. Balzari and V. Carassiti, Academic Press.
- 6. Elements of Inorganic Photochemistry, G.J. Ferraudi, Wiley.
- 7. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern.
- 8. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
- 9. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
- 10. Introductory Photochemistry, A. Cox

MCHE317: Medicinal Chemistry

Credit:4 (Four Lectures Per Week)

VI.M: 100

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR) factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR, Concepts of drug receptors. Elementary treatment of drug receptor interactions, Physicochemical parameters: lipophilicity, partition coefficient, electronic ionization constant, steric, Shelton and surface analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematica) activity parameters and redox potentials. Free Wilson derivations of equations excluded).

Dnit II

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacoki netic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinétics in drug, development process.

Unit III

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotic, biotransformation, significance of drug metabolism in medicinal chemistry.

Unit IV

Antineoplastic Agents

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, and 6-mercaptopurine. Recent development in carneer chemotherapy. Hormone and natural products.

Unit V

Antibiotics

Cell wall biosynthesis inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

Books suggested

1. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH.

2. Wilson and Gisvold's: Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ecl. Robert F. Dorge. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International:

4. Burger's Medicinal Chemistry and Drug Discovery, Vol-I, Ed. M.E. Wolff, John Wiley.

Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.

The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

MCHE318: Spectroscopy and Solid State Chemistry

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Electron Spin Resonance Spectroscopy

Principle and theory, Kramer degeneracy, g factor, electron-nuclear coupling (hyperfine structure), line shape and width, Mc Connell relationship, endor and eldor, electron-electron coupling. Techniques of measurement, application of ESR to organic free radicals and to transitional metal complexes (having and unpaired electron) including biological systems.

Unit II

Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-roatational Raman spectroscopy, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

Unit III

Microwave Spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect, nuclear and electron spin interaction and effect of external field.

Unit IV

Photoelectron Spectroscopy

Basic principles, photoelectric effect, ionization process, Koopman's Theorem, photoelectron spectra of simple molecules, ESCA, chemical information from ESCA, Auger electron spectroscopy-basic idea.

Unit V

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)

Definition, deduction of absolute configuration and octant rule for ketones.

Unit VI

Solid State Chemistry

(a). Solid State Reactions

General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of (b). Organic Solids, Fullerene, Molecular devices

Electrically conducting solids, organic charge transfer complex, organic metals, magnetism in organic materials, fullerenes and doped fullerenes, organic superconductors, molecular rectifiers, transistors, artificial

Books Suggested

1. Physical Method for Chemistry, R.S. Drago, Saunders Company.

2. Structural Method in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS

3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood. 4. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J. Martin, Heyden.

Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C.

LIST OF SELFSTUDY PAPERS IN HITT SEMESTER

MCHS319: Traditional Health Care System Of Uttarakhand Including Ayurvedic Medicine

M.M: 100

Study of Indigenous Traditional Drugs Botanical sources, clinical uses, chemical constituents, pharmacological action and authentication of various herbal Drugs. Introduction to Ayurvedic Dosage Forms Preparation and Standardization of Ayurvedic Preparation such as Asavas, Aristha, Avaleha, Churna...

MCHS320: Pesticide Chemistry

M.M: 100

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

Semester- IV

MCHC401: Chemistry of Natural Products

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule Structures of abietic acid and β -carotene.

Unit II

Alkaloids

Classification, Nomenclature, Isolation and structure of ephedrine, quinine.

Unit III

Steroids

Structural features of cholesterol and bile acids (without synthesis). Chemistry of testosterone, estrone and progestrone.

Unit IV

Pigments

(a) Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of cyanidin, and quercetin.

(b) Porphyrins

General Introduction of haemoglobin and chlorophyll. Chemistry of chlorophyll (without synthesis). Structure and synthesis of haem.

Unit V

Prostaglandins

Occurrence, nomenclature, classification, biogenesis and physiological effects Synthesis of Key intermediate, PGE2 and PGF2

Books Suggested

- 1. Natural Products: Chemistry and Biological Significance, J.Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
- 2. Organic Chemistry, Vol 2, I.L. Finar, ELBS.
- 3. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
- 4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
- 5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt. Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
- 6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers.
- 7. New Trends in Natural product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers

Then's Dunghiller

MCHL402: Laboratory Course

M.M:100

Credits:3(nine hrs per week)

I. Extraction of Organic Compounds from Natural Sources

- 1. Isolation of caffeine from tea leaves.
- 2. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
- 3. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported). 4. Isolation of nicotine dipicrate from tobacco.
- 5. Isolation of cinchonine from cinchona bark,
- 6. Isolation of piperine from black pepper.
- 7. Isolation of lycopene from tomatoes.
- 8. Isolation of -carotene from carrots.
- 9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of 10. Isolation of eugenol from cloves.
- 11. Isolation of limonene from citrus fruits.

II. Paper Chromatography

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.

III. Spectroscopy

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS)

IV. Spectrophotometric (UV/VIS) Estimations

- 1. Amino acids
- 2. Proteins
- 3. Carbohydrates
- 4. Cholesterol
- 5. Ascorbic acid
- 6. Aspirin
- 7. Caffeine

Books Suggested

- 1. Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman and GS Kriz,
- 2. Operational Organic Chemistry, A Laboratory Course, Second Edition, JW Lehman, Allyn & Bacon, Inc.
- Microscale Organic Experiments KL Williamson, DC Health & Co. Le Xington.
- Laboratory Manual of Organic Chemistry, RK Bansal, New Age International, Delhi.
- Introduction to Organic Laboratory Techniques (Third Edition), DL Pavia, GM Lampman and GS Kriz,
- 6. Operational Organic Chemistry, A Laboratory Course, Second Edition, JW Lehman, Allyn & Bacon, Inc.
- Microscale Organic Experiments KL Williamson, DC Health & Co. Le Xington.
- 8. Laboratory Manual of Organic Chemistry, RK Bansal, New Age International, Delhi.

MCHC403: Dissertation

Credits: 9 M.M:300

Project from parent institute/industry /Research Organizations. Project should be completed under the guidance of a faculty member in the same Department or Industry or research organization. In case of Industry / research organization one member of that body can also be included as project guide.

MCHC404: Inorganic Polymers

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Inorganic polymer synthesis, step-growth and step condensation synthesis of metal containing polymers. Condensation of functionalised metal containing species, condensation through bridged ligand coordination, bridging ligand formation during condensation, synthesis of main group condensation polymer

.Polycarboranes, polycarbosilanes, polythalocyanines, polysiloxanes. Chain polymerisations, radical and cationic polymerisations.

Unit III

Inorganic polymer characterization, methods of characterizing average molecular masses.

Glass transition temperature measurement, spectroscopic characterization specific to inorganic polymers, use of NMR and EPR in characterization of inorganic polymers, use of electronic, vibrational, Mossbauer spectroscopies in charaterization of inorganic polymers, visco-elasticity measurements. Crystall inity characterization.

Unit V

Polymer elastomers, inorganic dental polymers, adhesives, inorganic high temperature fluids and lubricants. Unit VIII Inorganic polymer conductivity, metal containing polymers, metal containing polymers in non linear optics,

Books suggested

Inorganic and Organometallic Polymers, Ronald D. Archer, Wiley VCH, 2001.

2. Inorganic Polymers, J. E. Mark et al., Prentice Hall, 1992.

MCHL405: Laboratory Course

M.M:100

Credits:3 (nine hrs per week)

- Spectrophotometric Determinations
 - (a). Manganese/chromium/vanadium in steel sample.
 - (b). Nickle/molybdenum/tungsten/vanadium/uranium by extractive Spectrophotometric method.
 - (c). Fluoride/nitrite/phosphate.
 - (d). Iron-phenanthroline complex; Job's Method of continuous variation.
 - (e). Zirconium-alizarin Red-S complex: Mole-ratio method.
 - (f). Copper-ethylene diamine complex: Slope -ratio method.
- Flame Photometric Determinations
 - (a). Sodium and Potassium when present together.
 - (b).Lithium/Calcium/barium/strontium.
 - (c).Cadmium and magnesium in tap water
- Nephelometric Determinations
 - (a). Sulphate
 - (b). Phosphate
 - (c). Silver
- Chromatographic separations: Paper or TLC and determination of Rf values:

 - (b). Silver, Lead and Mercury.
 - (c). Nickel, Magnesium, Cobalt and Zinc.

MCHC406: Advanced Quantum Chemistry

M.M: 100

Credit:4 (Four Lectures Per Week)

Unit I

Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock Theory

Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater-Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Roothan equation, Gaussian basis sets.

Configuration Interaction and MC-SCF

Introduction to CI; full and truncated CI theories, size consistency, Introductory treatment of coupled cluster and

Unit III

Semi-Empirical Theories

A review of the Huckel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MOPAC and AMI with hands on

Unit IV

Density Functional Theory

Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulation, N- and V- representabilities; review of the performance of the existing local (e.g. Slater Xa and other methods) and non-local functionals, treatment of

Unit V

Computer Experiments

Computer experiments using quantum chemistry- software packages such as GAUSSIAN/GAMESS/MOPAC and

Books Suggested

1. Modern Quantum Chemistry, N.S. Ostlund and a. Szabo, McGraw Hill.

2. Methods of Molecular Quantum Mechanics, R. Meweeny and B.T. Sutcliffe, Academic Press 3. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford.

4. Exploring Chemistry with Electron Structure Methods, J.B. Foresman and e. Frish, Goussian Inc.

MCHL407: Laboratory Course

M.M:100

Credits:3(nine hrs per week)

- · Determination of transport number.
- · Determination of liquid junction potential.
- Determination of the charge on colloidal particle.
- · Polarography.
- · Beer's law verification.
- Decomposition of potential determination.
- · Validity of Freundlich's adsorption isotherm.
- · Validity of Langmuir's adsorption isotherm.
- Determination of partial molar volume of solute.
- Determination of CMC of surfactants

LIST OF ELECTIVE PAPERS IN IVth SEMESTER

MCHE408: Green Chemistry

M.M: 100

Unit I. Green chemistry: History, need, and goals. Green chemistry and Sustainability. Dimensions of sustainability, Limitations/Obstacles in pursuit of the goals of Green Chemistry. Opportunities for the next generation of materials designers to create a safer future.

Unit II

Basic principles of Green Chemistry and their illustrations with examples.

- Prevention of waste/byproducts.
- Maximum Incorporation of the materials used in the process into the final product (Atom Economy): Green metrics
- Prevention/Minimization of hazardous/toxic products.
- Designing safer chemicals different basic approaches
- Selection of appropriate auxiliary substances (solvents, separation agents etc)
- Energy requirements for reactions—use of microwave, ultrasonic energy
- Selection of starting materials—use of renewable starting materials.
- Avoidance of unnecessary derivatization—careful use of blocking/protection groups.
- Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents.
- Designing biodegradable products.
- Prevention of chemical accidents.
- Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

Unit III

Examples of green synthesis/reaction:

- · Green starting materials
- Green reagents
- Green solvents and reaction conditions
- Green catalysis
- Green synthesis- Real world cases

(Traditional processes and green ones)

Synthesis of Ibuprofen, Adipic acid etc and selected examples from US Presidential Green

Chemistry

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Unit IV

Hazard assessment and mitigation in chemical industry

Future trends in Green Chemistry: Oxidation-reduction reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; Noncovalent derivatization. Biomass conversion, emission control. Biocatalysis

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Credit:4 (Four Lectures Per Week)

Books Suggested:

- 1. Green Chemistry: Theory and Practice. P.T. Anastas and J.C. Warner. Oxford University Press.
- 2. Green Chemistry: Introductory Text. M. Lancaster Royal Society of Chemistry (London).
- 3. Introduction to Green Chemistry. M.A. Ryan and M.Tinnesand, American Chemical Society (Washington).
- 4. Real world cases in Green Chemistry, M.C. Cann and M.E. Connelly. American Chemical Society (Washington).
- 5. Real world cases in Green Chemistry (Vol 2) M.C. Cann and T.P.Umile. American Chemical Society (Washington)

MCHE409: Modern Techniques of Chemical Analysis

M.M: 100

Credit:4 (Four Lectures Per Week)

UNIT-I

Spectrophotometry:

i) Introduction, fundamental laws of photometry, the electromagnetic spectrum and spectrochemical methods, UV/Visible instrumentation, absorption spectra, Beer-Lambert's Law, deviation from Beer-Lambert's Beer's Law, ii) Photometric Titrations:- Simultaneous spectrophotometric determination, differential spectrophotometry, titration curves and applications to quantitative analysis, iii) Molecular Fluorescence Spectroscopy:- Theory, relaxation processes, relationship between excitation spectra and florescence spectra, florescencent species, effect of concentration on florescence intensity, instrumentation and application of florescence methods.

UNIT-II

Atomic Spectroscopy:

Theory of flame photometer, intensities of spectral lines, selection of optimal working conditions, applications of flame photometry to quantitative analysis. The Theory of Atomic Absorption Spectroscopy (AAS), Origin of atomic spectra, line width effects in atomic absorption, instrumentation and its application, Atomic emission spectroscopy (AES) and the detailed description of the techniques of inductively coupled plasma AES (ICP-AES) and its instrumentation. Chemical and spectral interferences encountered in both techniques and how to overcome them.

UNIT-III

Electroanalytical Methods:

- a) Electrogravimetric methods:- i) Current-voltage relationship during electrolysis, operation of a cell at a fixed applied potential, costant current electrolysis, physical properties of electrolytic precipitates, chemical factors of electrolysis), apparatus and applications. iii) Spontaneous electrogravimetric analysis (internal applications.
- b) Coulometric Methods: i) Controlled potential Coulometry, instrumentation and applications. ii) Coulometric titrations, cell for coulometric titrations of coulometric titrations (neutralization, precipitation, and complex formation titrations), comparison of coulometric and volumetric titrations.

UNIT-IV

Polarographic Methods: General introduction: Theoretical measurements of classical polarography, polarographic measurements, polarograms, interpretation of polarographic waves, equation for polarographic (advantages and limitations), current variation with a dropping electrode, polarographic diffusion current, the and catalytic current, polarograms for mixtures of reactants, anodic waves and mixed anodic and cathodic waves, applications to inorganic and organic analysis

(a) Thermogravimatric analysis: Introduction, Factors affecting thermogravimetric curves, instrumentation, applications to inorganic compounds (analysis of binary mixtures i.e. Ca and Mg, TG curves of calcium oxalate, determination of Ca, Sr & Ba ions in the mixture, drying of sodium carbonate, analysis of clays and soils, decomposition of potassium hydrogen phthalate, oxidation of nickel sulphide, determination of titanium content of non-stoichiometric sample of titanium carbide).

(b) Differential thermal analysis: Introduction, Factors effecting DTA curves, instrumentation, applications, to inorganic compounds (thermal decomposition of mixtures of lanthanum-cerium and praseodymium oxalate, DTA decomposition for different magnesium carbonate samples, determination in ammonium nitrate, thermal decomposition for different magnesium carbonate samples, determination of uncalcined gypsum in plaster of

MCHE410: Computers And Biostatistics

M.M: 100

Credit:4 (Four Lectures Per Week)

Computers

Unit I

History of computer Simple model of computer and its working, input-output devices, computer languages and their hierarchy(low level and high level), Introduction of microcomputers, concept of operating system, computer networking, concept of OSI layers, Introduction of software(MS-Word, MS-Excel & Power point etc.)

Unit II

Introduction of C++ Programming Difference between C and C++, concept of OOP'S, basic data types and operators, sample programs, conditional statements(IF-ELSE, NESTED IF), concept of looping(for, while and dowhile), Introduction to arrays(single and double), classs and objects, function & function overloading, constructor and destructor, file handling.

Unit III

Internet and its working, Uniform resource locator(URL), World wide web, HTTP, Internet explorer, PDB, NRL-3D, BLAST & FASTA, Special software to align sequences, general DNA sequence data base, protein structure data base, genome project database, human mapping data base.

Biostatistics

Unit IV

Introduction and scope of Biostatistics Presentation of data: classification of data, Methods of collection of data, frequency distribution, graphical representation of data by histogram, frequency polygon, frequency curve and cumulative frequency curve. Central tendency and measures of dispersion, mean, median, mode and their properties, partition value, standard deviation and coefficient of variation, simple correlation coefficient and and independence of attributes.

Unit V

Testing of hypothesis Types of errors, power of test, test of significance based on normal distribution T-test for mean of population, difference of means of two normal population, chi-square test of goodness of fit, independent test test of variance of normal population F-test for variance ration, correlation and regression, latest square methods and its application, significance of coefficient of correlation, rank correlation curve fitting and sign test.

BOOKS SUGGESTED

1.Information technology-D.P.Curtin, Tata McGraw Hill, New Delhi.

2.Guide to Medical Informatics, The Internet & Telemedicine-E Coiera, Amold Publishers, USA

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MCHE411:Environmental Chemistry

M.M: 100

Credit:4 (Four Lectures Per Week)

UnitI

Environment

Introduction, composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Bio distribution of elements.

Unit II

Atmosphere

Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals chlorofluorohydrocarbons. Analytical methods for measuring air

Unit III

Soils

Composition, micro and macro nutrients, Pollution of fertilizers, pesticides and metals.

Unit IV

Hydrosphere

Aquatic pollution- inorganic, organic, pesticides, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters-dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards. Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.) residual chloride and chlorine demand.

Environmental Toxicology

Introduction; threshold limiting value (TLV); Toxicity and control of toxicants-- Nonmetallic compounds, asbestos, organic compounds, endocrine disrupters, persistent organic pollutants (POP's), polychlorinated biphenyls (PCB's), dioxins, pesticides, phthalates, heavy metals- As, Hg, Cd, Pb..

Books suggested

- Environmental Chemistry, S.E. Manahan, Lewis Publishers.
- Environmental Chemistry, Sharma and Kaur, Krishna Publishers.
- Environmental Chemistry, A.K. De, Wiley Eastern.
- Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern.
- Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
- 6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
- Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Environmental Chemistry, C. Baird, W.H. Freeman.

MCHE412: Chemistry of Macromolecules

M.M: 100

Credit:4 (Four Lectures Per Week)

UNIT-I

The science of macromolecules, Importance of macromolecules / polymers, basic concepts of polymers viz. monomers, repeat units, degree of polymerization, classification of polymers on the basis of molecular weight and special arrangement viz. linear, branched and network polymers. Types of macromolecules (synthesized and natural), polymerization by condensation and addition reactions only. Molecular forces and chemical bonding in simple molecules and macromolecules and their effects on the physical properties. Polymer solutions, criteria for polymer solubility, conformations of dissolved polymer chains. Different models for describing the size and shape of dissolved macromolecules, configuration and conformation of macromolecules.

UNIT - II

Thermodynamics of polymer solutions, thermodynamics of simple liquid mixtures, ideal solutions, regular solutions, lattice model of solutions (Flory - Huggins Theory), Flory - Krigbaum theory for dilute polymer solutions. Phase separation in polymer solutions involving binary polymer – solvent systems, ternary systems and multi - component systems. Fractionation of polymers by different techniques, theory of swelling of cross -UNIT - III

Measurements of molecular weights and size of macromolecules by osmotic pressure measurement, light scattering method, diffusion measurement, sedimentation and ultracentrifuge methods and viscosity methods. Molecular weights of macromolecules viz., number average and weight average molecular weights and related

Rheology and Mechanical Properties of Polymers: Brief introduction to rheology and mechanical properties of polymers, phenomena of viscous flow, kinetic theory of ribber elasticity, amorphous polymers and practical importance of their aggregation states, viscoelasticity (experimental and dynamic method), general mechanical models for an amorphous polymer, molecular structure and viscoelasticity. The glassy state and glass transition

1. Mechanical strength of polymers: Mechanical strength and life time of polymer mechanism of polymer fracture, effect of various factors on the mechanical properties of polymers (effect of size and shape, effect of

2. Polyelevtrolytes: The water soluble charged polymers and their applications. Ionomers (ion containg polymers) conducting polymers solid polymer electrolytes, mechanism of conductivity, polymer colloids and their applications in commercial and industrial formulations (adhesives, coating, paper, pharmaceutical and medical applications), polymer microgels, biomedical polymers. Polymers in combating environmental pollution and as

- 1. Text Book of Physical Chemistry: G.M. Barrow
- 2. Text Book of Polymer Chemistry: Billmeyer 3. Polymer Chemistry: P.J. Flory
- 4. Physical Chemistry of Polymers: A Tagger
- 5. Physical Chemistry of Macromolecules: C. Tanford
- 6. Introduction to Polymer Science: V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar

LIST OF SELFSTUDY PAPERS IN IVth SEMESTER

MCHS413: Analytical Chemistry

M.M: 100

UnitI

Introduction

Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations-dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

Unit II

Errors

Determinate and indeterminate errors, minimization of determinate errors, random distribution of indeterminate Unit III

Statistical data analysis

Accuracy and precision, significant figures and computations, mean and standard deviation, distribution of random errors, reliability of results, confidence interval, comparison of results, comparison of means of two samples, paired t-test, number of replicate determinations and its use, correlation and regression, linear regression,

Application of analytical chemistry in the study of water and soil pollutions, analysis of fuel, body fluids and

- Analytical Chemistry, G.D. Christian, J. Wiley.
- Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W.B. Saunders.
- 4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
- 5. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders. 6. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
- 7. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
- 8. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern. 9. Handbook of Instrumental Techniques for Analytical Chemistry, F.

MCHS414: Titrimetric Analysis

M.M: 100

Unit I

Fundamental of volumetric analysis Methods of expressing concentrations, primary and secondary standards. Neutralization reactions: Theory of indicators and neutralizations indicators.

Unit II

Oxidation-reduction titration Principle of oxidation reduction filtrations, redox indicators & their use in pharmaceutical analysis. Precipitation titration: Theory of precipitation titrations and use of adsorption indicators.

Unit III

Complexometric titrations Complexometric methods using EDTA, principle of complexometric titrations,

Unit IV

Nonaqueous titrations General discussion and principle of titrations in non-equeous media, aprotic, protophilic, protogenic and amphiprotic solvents. Titrations with perchloric acid, potassium methoxide and tetrabutyl

BOOKS SUGGESTED

- 1. A. H. Becket and J. B. Stenlake, Practical Pharmaceutical Chemistry, Part I, 4th ed., CBS Publishers & Distributors, New Delhi, 1997.
- 2. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney Vogel's Text Book of Quantitative Chemical Analysis
- 3. A. Keneth & A. Connors, A Text Book of Pharmaceutical Analysis, 3rd ed., Wiley Interscience Singapore,