DAVANGERE UNIVERSITY
Shivagangothri, Davangere – 577 007

POST-GRADUATE PROGRAMME
Master of Science (M. Sc.) in Chemistry

Choice Based Credit Scheme (CBCS) Syllabus
2016-17 onwards

DoS in Chemistry, Davangere University,
Shivagangothri, Davangere – 577 007

DAVANGERE UNIVERSITY
SHIVAGANGOTHRI

DEPARTMENT OF CHEMISTRY

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PROCEEDINGS OF THE PG-BoS MEETING HELD ON 28-05-2018

Chairman welcomed the board members for attending the BoS meeting of Department of Chemistry. Exhaustive discussions were held by the board members on course structure and then syllabus content for both Post-Graduate and Undergraduate Chemistry. The following resolutions were made and board members authorised the Chairman to hand over the same to Registrar, Davangere University.

01. Minor changes in Undergraduate Chemistry syllabus was made and it was resolved to incorporate minor changes in the syllabus.

02. It was resolved to keep the same syllabus for Post-Graduate Chemistry for the academic year 2018-19.

03. The board has formulated the Course Regulations, Structure and Syllabi for One year programme of PG Diploma in Analytical Chemistry.

04. List of examiners was also approved by the board members.

BoS Members	Name of the Institution	Signature
Prof. K.M. Mahadevan	Kuvempu University	
Prof. J. Seetharamappa	Karnataka University, Dharwad	Absent
Dr. K.N. Mohan	University of Mysore, Mysuru	Absent
Smt. B.S. Usha	SJM College, Chitradurga	
Smt. Shobha A Dalawayi	Govt. Science College, Chitradurga	
Dr. Sairabanu A Farokhi	Govt. First Grade College, Davangere	
Shri. H. Basavarajappa	DRM Science College, Davangere	

Chairman
Board of Studies in Chemistry

DAVANGERE UNIVERSITY

Shivagangotri, Davangere-577 002

POST-GRADUATE PROGRAMME - Choice Based Credit Scheme (CBCS)

❖ **Master of Science (M.Sc.,) in Chemistry**

SYLLABUS: 2016-2017

Structure, Course Titles, Workload & Credits

Course Number	Theory/ Practicals	Workload Per Week	FIRST YEAR		SECOND YEAR	
			Semester-I	Semester-II	Semester-III	Semester-IV
			Honours' Degree		*Master's Degree*	
I	Core	Theory-4	Inorganic Chemistry-I	Inorganic Chemistry-II	Organometallic Chemistry	Coordination & Bioinorganic Chemistry
II	Core	T-4	Organic Chemistry-I	Organic Chemistry-II	Reaction Mechanisms &Natural Products	Organic Synthetic Methods
III	Core	T-4	Physical Chemistry-I	Physical Chemistry-II	Radiation & Photochemistry	Chemical Dynamics & Catalysis
IV	Core	T-4	Molecular Spectroscopy-I	Molecular Symmetry & Spectroscopy-II	Principles of Analytical Chemistry	Project Work*
Course Related Practicals	Practicals-1	P-4	*Lab-1.1: Inorganic Chemistry-I*	*Lab-2.1: Inorganic Chemistry-II*	*Lab-3.1: Inorganic Chemistry-III*	*Lab-4.1: Inorganic Chemistry-IV*
	Practicals-2	P-4	*Lab-1.2: Organic Chemistry-I*	*Lab-2.2: Organic Chemistry-II*	*Lab-3.2: Organic Chemistry-III*	*Lab-4.2 Organic Chemistry-IV*
	Practicals-3	P-4	*Lab-1.3: Physical Chemistry-I*	*Lab-2.3: Physical Chemistry-II*	*Lab-3.3: Physical Chemistry-III*	*Lab-4.3: Physical Chemistry-IV*
	Practicals-4	P-4	*Lab-1.4: Applied Analysis-I*	*Lab-2.4: Applied Analysis-II*	*Lab-3.4: Analytical Chemistry-I*	*Lab-4.4: Analytical Chemistry-II*
TOTAL NO. OF HOURS/CREDITS		T-16+P-16 = 32 Hours	*T-16 Credits +P-16 (8 Credits) = 24 Credits*	*T-16 Credits +P-16 (8 Credits) = 24 Credits*	*T-16 Credits +P-16 (8 Credits) = 24 Credits*	*T-16 Credits +P-16 (8 Credits) = 24 Credits*

* **Project Work** = 100Marks(Of which ,75Marks for Dissertation and 25Marks for Presentation at the Viva-Voce Exam)

Skill Development Courses (with Test & Certificate at the Institution Level)				*Interdisciplinary Course* (Exam conducted by the University)	(Additional Interdisciplinary Course) *Option to Students*
Mandatory Courses	+ 4 Hours	Functional & Communicative English	Computer Basics & Applications to Chemistry	1. **Solid State Chemistry** 2. **Environmental Chemistry**	Subject from Other than Parent Discipline/Science/Non-Science
Socially Relevant Credit Audit Courses (Based on Lecture Series & Workshops) (No Exam will be conducted but Credits will be entered in the IV-Semester Mark Card)					
Compulsory Skill Development	+ 2 Hours	Basic Laws & Legal Awareness	Socially Relevant Issues	Administration & e-Governance	Personality Development

DAVANGERE UNIVERSITY

COURSES HAVING FOCUS ON EMPLOYABILITY/ ENTREPRENEURSHIP/ SKILL DEVELOPMENT

Course Code	Title of the Paper	Activities with direct bearing on Employability/ Entrepreneurship/ Skill development
Ch 1.1	INORGANIC CHEMISTRY-I	Employability in teaching
ChL1.1	INORGANIC CHEMISTRY-I	Basic Laboratory skills in preparation , separation and purification
Ch 1.2	ORGANIC CHEMISTRY-I	Employability in teaching profession and skill in understanding the chemical reactions.
ChL 1.2	ORGANIC CHEMISTRY-I	Skill development in chemical analysis and employability in teaching profession.
Ch 1.3	PHYSICAL CHEMISTRY-I	Employability in industries and teaching profession
ChL 1.3	PHYSICAL CHEMISTRY-I	Skill development in electro-analytical methods
Ch 1.4	MOLECULAR SPECTROSCOPY-I	Skill development in various spectroscopic techniques.
ChL 1.4	APPLIED ANALYSIS I	Skill development on analytical techniques and employability in various chemical/pharmaceutical industries.
Ch 2.1	INORGANIC CHEMISTRY -II	Employability in academic institutions and skills in separation of inner transition elements
ChL 2.1	INORGANIC CHEMISTRY -II	Analytical skills and estimation , separation of metals via semi-micro qualitative analysis
Ch 2.2	ORGANIC CHEMISTRY-II	Employability in various chemical industries, Entrepreneurship in establishing various chemical industries.
ChL 2.2	ORGANIC CHEMISTRY-II	Employability in pharmaceutical industries.
Ch 2.3	PHYSICAL CHEMISTRY-II	Employability in Teaching Profession
ChL 2.3	PHYSICAL CHEMISTRY-II	Employability in various chemical industries and teaching profession
Ch 2.4	MOLECULAR SYMMETRY AND SPECTROSCOPY-II	Skill development on various spectroscopic techniques.
ChL 2.4	APPLIED ANALYSIS-II	Skill development on analytical techniques and employability in various chemical/pharmaceutical industries.
Ch 3.1	ORGANOMETALLIC CHEMISTRY	Employability in academic and industries. Skills to apply transition metal complexes as industrial catalysts
ChL 3.1	INORGANIC CHEMISTRY –III	Skills in preparation and analysis of transition metal complexes and employability in pharmaceuticals
Ch 3.2	REACTION MECHANISMS AND NATURAL PRODUCTS	Employability in pharmaceutical industries and Teaching Profession
ChL 3.2	ORGANIC CHEMISTRY-III	Employability in chemical industries.
Ch 3.3	RADIATION AND PHOTOCHEMISTRY	Employability in industries.
ChL 3.3	PHYSICAL CHEMISTRY-III	Employability in various R&D laboratories.
Ch 3.4	PRINCIPLAS OF ANALYTICAL CHEMISTRY	Skill development in various analytical techniques.
ChL 3.4	ANALYTICAL CHEMISTRY-I	Employability in different analytical chemistry labs and entrepreneurship in analytical chemistry lab/industry
Ch 4.1	COORDINATION AND BIOINORGANIC CHEMISTRY	Critical thinking and employability in academic and bio-pharmaceutical /medicinal industries
ChL 4.1	INORGAIC CHEMISTRY-IV	Research skills in analytical industries and employability in R &D of institutions and industries

Ch 4.2	ORGANIC SYNTHETIC METHODS	Research skill, employability in industries and research organization.
ChL 4.2	ORGANIC CHEMISTRY-IV	Employability in various chemical industries and research Institute.
Ch 4.3	CHEMICAL DYNAMICS AND CATALYSIS	Employability in teaching and entrepreneurship in Industries.
ChL 4.3	PHYSICAL CHEMISTRY-IV	Employability in different analytical and electro-analytical laboratories.
Ch 4.4	CHEMICAL DYNAMICS AND CATALYSIS	Employability in teaching and Industries.
ChL-4.4	ANALYTICAL CHEMISTRY-IV	Employability in various kinds of analytical chemistry research laboratories and related industries.
-	Project Work/Dissertation	Ability to do independent research work in chemistry and employability in chemical industry.

FIRST SEMESTER SYLLABI OF M. Sc. PROGRAMMES IN CHEMISTRY

THEORY PAPERS

THEORY-1:
Ch-1.1: INORGANIC CHEMISTRY-I **56Hrs**

UNIT I: 14 hrs

Ionic bond: properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds, hydration energy and solubility of ionic solids.

Covalent bond: valence bond theory, resonance, hybridisation, Bent's rules and enregetics of hybridization, Deduction of molecular shapes – VSEPR theory.

M.O.theory, application to homo- and hetero-diatomic and -triatomic molecules.

UNIT II: 14 hrs

Alkali and alkaline earth metal complexes of crown ethers, cryptands and calixarenes and their biological significance.

Halogens and Noble gas chemistry –interhalogens, psuedohalogens, polyhalide ions, oxyhalogen species, xenon oxides and fluorides. Oxy- and peroxy acids of N, P and S. Graphitic compounds, carbides, pure silicon, silica and silicates, zeolites.

UNIT III: 14 Hrs

Theories of acids and bases – Bronsted and Lewis acids and bases, Lux-Flood theory, gas phase vs. solution acidity, solvent leveling effects, hardness and softness, HSAB concept. super acids. Reactions in non-aqueous media: Liquid ammonia, anhydrous sulphuric acid, glacial acetic acid, anhydrous HF, bromine trifluoride, liquid sulphur dioxide and dinitrogen tetroxide. Reactions in molten salts.

UNIT IV: 14 Hrs

Sampling techniques, preparation of samples for analysis. Nature of errors, statistical treatment of errors, the t- and F-tests, significant figures, rejection of data.

Precipitation phenomena: precipitation from homogeneous solutions, organic precipitants in inorganic analysis. Solvent extraction of metal ions, nature of extractant, distribution law, partition coefficients, types of extractions and applications.

Theories of redox indicators, titration curves, feasibility of redox titrations.

Chelometric titrations- titration curves with EDTA, feasibility of EDTA titrations, indicators for chelometric titrations, selective masking and demasking techniques, industrial applications of masking.

References:

1. J.E Huheey, Keiter, Keiter and Medhi: Inorganic Chemistry (4th ed.), Pearson Education, 2006.
2.Shriver, Atkins and Langford : Inorganic Chemistry (3rd edn.) OUP, 1999.
3.J.D.Lee: Concise Inorganic Chemistry, (5th edn.) Blackwell Science, 2000.
4.B.E.Douglas, D.McDaniel & A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5.W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.

THEORY-2:
Ch-1.2: ORGANIC CHEMISTRY-I 56HRS

UNIT I 14 Hrs

Nature of Bonding in Organic Molecules: Localized and delocalized bonding**:** Conjugation, cross conjugation, resonance, hyper-conjugation and tautomerism. Aromaticity in benzenoid and non-benzenoid molecules, Huckel rule, alternant and non-alternant hydrocarbons, Homo-aromatic and anti-aromatic systems. Annulenes and hetero-annulenes.

Bonds weaker than covalent: Addition compounds, crown ether complexes, cryptands, inclusion compounds, catenanes, valence isomers, fluxional molecules.

Acids and Bases: Introduction to acids and bases, Bronsted-Lowry concept, organic acids and bases, pKa and pH, effect of solvent on acid and base strength, effect of structure of organic compound on acid and base strength, Lewis acids and bases, acid-base reactions.

UNIT-II 14 Hrs

Reaction Intermediates: Generation, structure, stability, reactivity and detection of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Singlet oxygen-generation and reactions with organic molecules.

Methods of Determining Reaction Mechanism: Kinetic and non-kinetic methods, Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, kinetic evidences and kinetic isotopic effects.

UNIT III: Stereochemistry 14Hrs

Optical Isomerism: Conformation and configuration of molecules, projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations. Absolute configuration(D,L) and (R,S) systems. Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity.11hrs

Geometrical Isomerism: Cis-trans isomerism resulting from double bonds, monocyclic compounds & fused ring systems. E,Z-notations, den. of configuration of geometrical isomers, syn & anti isomers.

UNIT IV: Carbohydrates 14Hrs

Configuration and conformation of monosaccharides, Chemistry o f important derivatives of monosaccharides-ethers, esters, acetals, ketals, deoxysugars, aminosugars, Structure of disaccharides-maltose, cellobiose and sucrose. General methods of structural degradation of polysaccharides-methylation, partial hydrolysis, periodate oxidation, Smith degradation and alkaline degradation techniques. Structures of cellulose, chitin, starch and glycogen.

References:

1.Organic Chemistry-P.Y.Bruice (Pearson Education Pvt. Ltd.,New Delhi),2002.
2.Stereochemistry,Conformation and Mechanism-P.S.Kalsi (Wiley Eastern,New Delhi)1993.
3.Stereochemistry of Carbon Compounds-E.L.Eliel (Tata McGraw Hill, New. Delhi) 1994.
4.Advanced Organic Chemistry-Reactions, mechanisms & structure-J.March(Wiley, NY)2000.
5.Organic Chemistry-Vol. -1,2 &3-Mukherji, Singh and Kapoor. (Wiley Eastern,) 1994.
6.A guide book of mechanisms in Organic Chemistry-P.Sykes (Orient- Longman) 1985.
7.Organic Chemistry-R.T. Morrison and R.N. Boyd (Prentice Hall, New Delhi) 1994.
8.Organic Chemistry 4th Edn.–S.H. Pine et al (McGraw-Hill, London) 1987.
9.Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.
10.Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.
11.A Text book of Organic Chemistry-Tewari, Vishnoi and Mehrotra (Vikas, New Delhi)1998.
12.A Text book of Organic Chemistry-3rd Edn.-R.K. Bansal, (New Age, New Delhi) 1997.
13.Organic Chemistry-3rd Edn- F.A. Carey (Tata McGraw Hill, New Delhi) 1996.

THEORY-3:

Ch-1.3: Physical Chemistry-I 56hrs

UNIT – I : 14 hrs

Chemical Thermodynamics : A brief resume of laws of thermodynamics (combined form of 1st and 2nd laws), entropy as a measure of unavailable energy, Concept of fugacity and free energy, entropy and free energy changes and spontaneity of processes. Variation of free energy with T & P, Maxwell's relations, thermodynamics equations of state, limitations of Van't Hoff`s equation, Nernst heat theorem & its applications.Third law of thermodynamics, determination.of third law of entropies. 5 hrs

Application of thermodynamics : Entropy and free energy of mixing, partial molar quantities, partial molar volume and free energy (chemical potential), their significance and determinations. Gibbs-Duhem and Duham-Margules equations.

Thermodynamics of non-ideal solutions -Activity, activity coefficient-standard states.

Thermodynamics of ideal solutions - deductions of laws of Raoult ebullioscopy, cryoscopy and osmotic pressure. Quantitative treatment of Le-Chatelier principle

UNIT - II : 14 hrs

Phase Rule:Application to 3-component systems. An introduction to 4-component system. 3 hrs

Chemical Kinetics: Complex reactions- parallel, consecutive and reversible reactions. Chain reactions (H_2-halogen reactions). Branched chain reactions- general rate expression, explosion limits Photochemical (H_2-halogen reactions) and oscillatory reactions.

Reactions in solution: Ionic reactions - salt and solvent effects. Substituent effects on the rates of reactions - Hammett and Taft equations, linear free energy relationships.

Theories of reaction rates: Activated complex theory and its applications to reactions in solution. An introduction to study of fast reactions.

UNIT-III : 14hrs

Catalysis: Homogeneous catalysis-equilibrium and steady state treatments, activation energies of catalysed reactions. Acid-base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed reactions-Michaelis-Menten equation.Effect of pH, temperature&inhibitors

Surface reaction kinetics: A review of adsorption isotherms, uni- and bi-molecular reactions. multilayer adsorption-BET equation- application in surface area determination. Harkin–Jura equation-application. Desorption & heterogeneous catalysis–catalytic activity at surfaces, semiconductor catalysis, n-&p-type.Mechanism of surface reactions.Industrial application of catalysts.

UNIT-IV : 14 hrs

Electrochemistry of solutions: Ionic atmosphere, factor effecting conductance, Debye-Huckel-Onsager equation of conductivity and its validity. Walden`s rule and its application. Conductance minima, Concept of Ionic strength, Debye-Huckel limiting law (DHL), modifications to DHL-Types, qualitative tests and verification of DHL. Bjerrum theory of ion association-triple ion and significance.

Electroanalytical Techniques: Polarography- Theory, techniques and types. Applications in organic analysis, antibiotics containing nitro group, in pharmacy and parmocology and in analysis of agrochemicals. Theory, techniques and applications of coulometry, amperometry, cyclic voltammetry. Introduction to chronopotentiometry and chronoamperometry and electrogavimetry.

REFERENCES :

1. Physical Chemistry, 5th Ed., - Atkins (ELBS) 1995.
2. Physical chemistry – G. M. Barrow (McGraw Hill, Int. St. Ed) 1988.
3. Fundamentals of Physical Chemistry – Maron and Lando (Collier Macmillan) 1974.
4. Thermodynamics for Chemists - S. Glasstone (East-west) 1973.
5. Themodynamics - Rajaram and Kuriokose (East-West) 1986.
6. Chemical Kinetics - K.J.Laidler (Harper and Row) 1987.
7. Electrochemistry - Glasstone, Affiliated to East-west press, 1942.
8. Principles and Applications of Electrochemistry–Crow (Chapman hall, London) 1988

THEORY-4:

Ch-1.4: MOLECULAR SPECTROSCOPY-I 56hrs

UNIT -I 14 Hrs

Unifying Principles -Electromagnetic radiation, dual nature, regions of the spectrum, interaction of electromagnetic radiation with matter - absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Natural line width and broadening, intensity of spectral lines. Rotational, vibrational and electronic energy levels, selection rules.

Microwave Spectroscopy- The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond lengths, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

Vibrational Spectroscopy: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO_2 & H_2O).

UNIT –II : 14 Hrs

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation, sample handling techniques, FTIR Spectroscopy. Far IR region - metal-ligand vibrations, normal co-ordinate analysis.

Raman Spectroscopy: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, vibrational - rotational Raman spectra, selection rules, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman Spectrometer – instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - H_2O, N_2O & CO_2 molecules). An introduction to Resonance Raman Spectroscopy.

UNIT –III : 14 Hrs

Application of infrared spectroscopy in the structural study-identity by fingerprinting and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance.

Polarimetry: Plane polarized light, instrumentation, acid-catalyzed muta rotation of glucose, inversing of cane sugar-relative strengths of acids. Optical rotatory dispersion &circular dichroism–introduction, selection rules, deduction of absolute configuration, octant rule for ketones and cotton effect.

UNIT - IV: Nuclear Magnetic Resonance Spectroscopy 14 hrs

Magnetic properties of nuclei, theory and measurement techniques, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, A_2B_2), spin decoupling; effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents, solvent effects and Nulear Overhauser Effect. High resolution ^{1}H NMR. Applications of NMR spectroscopy in structure elucidation of simple organic and inorganic molecules. ^{1}H NMR in the structural study of complex organic compounds. Pulse techniques in NMR, two dimensional and solid state NMR.Use of NMR in Medical diagnostics.

REFERENCES:

1.Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill)2001.
2. Organic Spectroscopy-3rd ed.-W.Kemp (Pagrave Publishers, New York), 1991.

3. Spectrometric Identification of Organic Compounds-Silverstein, Bassler&Monnill(Wiley)1981.

Practicals:

1.Ch.Lab-1.1: Inorganic Chemistry -I
2.Ch.Lab-1.2: Organic Chemistry -I
3.Ch.Lab-1.3: Physical Chemistry-I
4.Ch.Lab-1.4: Applied Analysis -I

Note:Practicals are based on theory Papers exept Ch.Lab-1.4

SECOND SEMESTER SYLLABI OF M.Sc. CHEMISTRY

THEORY PAPERS:

THEORY-1:
Ch-2.1: INORGANIC CHEMISTRY -II 56Hrs

Unit I: 14 Hrs

Chemistry of higher boranes, classification, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of B_5H_9, $B_{10}H_{14}$ and $B_nH_n^{2-}$. carboranes and metallocarboranes. Cyclophosphazenes, phosphazene polymers, P-O and P-S cage compounds. S-N compunds : binary sulphur nitrides- S_4N_4, S_2N_2 and $(SN)_x$. Borazines and boron nitride, Isopoly and heteropoly acids of transition metals.

Unit II: 14 Hrs

Coordination numbers 2-10 and their geometry, crystal field theory of coordination compounds, d-orbital splittings in octahedral, square planar and tetrahedral fields, spectrochemical series, Jahn-Teller effect.

Structural evidences for ligand field splittings – hydration, ligation and lattice energies, site preference energies. MO theory of coordination compounds- MO energy level diagrams for octahedral and tetrahedral complexes.

Stepwise and overall formation constants, factors affecting stability of metal complexes, determination of binary formation constants by pH-metry and spectrophotometry.

Unit III: 14 Hrs

Metal Pi-acceptor complexes: metal carbonyls – preparative methods, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, magnetic and X-ray evidences of structures, M.O.representation of bi- and tri-nuclear carbonyls,. reactions metal carbonyls. Metal carbonylates and carbonyl halides – preparation and important reactions. Chemistry of metal nitrosyls – preparation, structure and bonding; dinitrogen and dioxygen complexes. Metal-metal bonding in carbonyls and halides, evidences for M-M bonding, factors favouring M-M bond formation. Metal clusters- bi-, tri-, tetra-, penta- and hexanuclear metal clusters, bonding in metal clusters. Zintl ions and Chevrel phases.

Unit IV: 14 Hrs

Methods of reduction of oxide ores, Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, effect of complexation on potential.

Trends in oxidations states, stereochemistry and ionic sizes of metals, comparison of 3d, 4d and 5d series by taking Ti subgroup as example. Lanthanides and actinides: electronic structure, oxidation states, extraction and separation of lanthanides, stereochemistry, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide complexes as NMR shift reagents. Comparison with d-block ions.

References:

1.J.E Huheey, E.A..Keiter, R.L.Keiter & O K Medhi: Inorganic Chemistry (4th edn.), Pearson, 2006.
2.Shriver, Atkins and Langford : Inorganic Chemistry (3rd edn.) OUP, 1999.
3.J.D.Lee: Concise Inorganic Chemistry, (5th edn.) Blackwell Science, 2000.
4.B.E.Douglas, D.McDaniel &A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5.W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.

THEORY-2:

Ch-2.2: ORGANIC CHEMISTRY-II **56Hrs**

UNIT I 14 Hrs

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions-S_N1, S_N2 and S_Ni. Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions, neighbouring group participation and anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions.

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms-S_E1, S_E2 and S_Ei mechanism. Electrophilic substitution reactions accompanied by double bond shifts.

Aromatic Electrophilic and Nucleophilic Substitution Reactions: Mechanism of aromatic electrophilic substitution reactions, Arenium ion mechanism, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems. Mechanism of Vilsmeir-Haack reaction, Pechmann reaction and Fries rearrangement. Mechanisms of aromatic nucleophilic substitution reactions- S_NAr, S_N1 & aryne mechanism. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement.

UNIT II 14 hrs

Free Radical Reactions: Types, mechanisms of free radical substitution reactions & neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead. Reactivity of attacking radical. Effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann & Hunsidiecker reactions.

Elimination Reactions: Discussions of E1, E2, E1cB and E2cB mechanisms. Orientation during elimination reactions. Saytzeff and Hofmann rules. Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium.

Pyrolytic Eliminations: Mechanisms of pyrolysis of esters of carboxylic acids. Chugaev reactions, Hofmann degradatrion, Cope elimination and xanthate pyrolysis. 4 hrs

UNIT III 14 hrs

Formation and Hydrolysis of Esters: Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis-$A_{AC}2$, $B_{AC}2$, $A_{AC}1$ & $A_{AL}1$ mechanism. Transesterification. 4 hrs

Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclicmechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, carboxylic acids and amines. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds. 6 hrs

Addition to Carbon-Hetero Multiple Bonds: Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformasky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions. 4 hrs

UNIT IV : Chemistry of Heterocyclic Compounds: 14hrs

Introduction, saturated and unsaturated heterocycles, three membered heterocycles - structure, reactivity, synthesis and reactions of aziridines, epoxides, episulfides, diaziridines, oxaziranes and diazirines, five membered simple and fused heterocycles-synthesis & reactions of derivatives of furan, pyrrole, thiophene &indole. Six membered heterocycles-synthesis & reactions of derivatives of pyridine. Biologically important heterocycles.

References:

1.Organic Reactions and Their Mechanisms- P.S. Kalsi (New Age, New Delhi),1996.
2.Advanced Organic Chemistry 4th Edn- J. March (Wiley, NY) 2000.
3.Organic Reaction Mechanisms- Bansal (Tata McGraw Hill, New Delhi) 1978.
4.Organic Chemistry-Vol. –I & II-Mukherji, Singh and Kapoor. (Wiley Eastern, New Delhi) 1985.
5.Mechanism and Theory in Organic Chemoistry-Lowry and Richardson Harper and Row, 1987.
6An Introduction to the Chemistry of Heterocyclic Compounds-Acheson (Wiley –Eastern) 1987.
7.Heterocyclic Chemistry-J. Joule & G. Smith, (Van-Nostrand, ELBS), 1978.
8.Reaction Mechanisms in Organic Chemistry-Mukherji, Singh and Kapoor (McMillan) 1978.
9.Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.

THEORY-3:

Ch-2.3: PHYSICAL CHEMISTRY-II **56Hrs**

UNIT - I : Quantum Chemistry **14 hrs**

A brief resume of black body radiation, and atomic spectra-Bohr's theory of hydrogen atom. Photoelectric and Compton effects, de-Broglie concept, uncertainty principle, operators, matrix representation and commutation relationships, Schroedinger equation, significance and characteristics of wave function, eigen functions and eigen values. Probabilities, normalisation and orthogonality. Postulates of quantum mechanics. Solution of Schroedinger wave equation for exactly solvable problems such as particle in a box (1D and 3D), particle in a ring, harmonic oscillator, rigid rotor and hydrogen atom (separation of r,θ,ϕ equations and their solutions), Quantum numbers and their characteristics, orbital diagrams.

UNIT–II: **14hrs**

Need of approximate methods in quantum chemistry. Approximate methods of solving Schroedinger equation for problems of chemical interest - variation and perturbation methods. Application of variation method to H & He atoms, the structure of many electron systems/atoms (secular equations & determinants), Spin-orbit interaction, antisymmetry and Pauli exclusion principle. Angular momenta (commutations, relations, operators), Term symbols, Russell-Saunders terms and coupling schemes, Slater orbitals and SCF method for many electron systems.

Molecular wave functions: Born-Oppenheimer approximations. Covalent bond –valence bond and molecular orbital approaches with comparisons. MO theory applied to homonuclear and heteronuclear diatomics by LCAO methods, correlation diagrams, non-crossing rule.

UNIT -II : **14 Hrs**

Theory of directed valence-hybridization and geometry of molecules in terms of molecular orbitals (bond angle, dihedral angle), localised and delocalised molecular orbitals.

Conjugated and aromatic molecules: Huckel molecular orbital (HMO) theory of linear conjugated systems (ethene, allyl & butadiene systems) and aromatic molecules (benzene as an example). Calculation of delocalization energies, bond order & charge density. An introduction to Extended Huckel Theory and its simple applications (as a means to explain modern theoretical methods: Semi empirical and ab initio SCF methods).

UNIT - III : Statistical and irreversible thermodynamics **14 hrs**

Statistical Thermodynamics : Micro and macrostates, phase space and ensembles. Concept of distribution - thermodynamic probability and most probable distribution - Maxwell-Boltzmann distribution law. Maxwell`s distribution of molecular velocities. Maxwell-Boltzmann statistics and applications, Bose-Einstein and Fermi-Dirac statistics. Partition functions - definitions and separations, evaluation of translational, rotational, vibrational and electronic partition functions for monoatomic, diatomic and polyatomic gaseous molecules. Calculations of thermodynamic functions and equilibrium constant in terms of partition functions, entropy of monoatomic gas - Sackur-Tetrode equation, comparison of 3rd law and statistical entropies. Heat capacity behaviour of solids 9hrs.

Irreversible Thermodynamics- Thermodynamic criteria for non-equilibrium states. Entropy production in chemical reactions. Transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations. Microscopic reversibility and Onsager`s reciprocity relations. Electrokinetic phenomena and thermoelectricity. Irreversible thermodynamics for biological systems and non-linear regime 5hrs

REFERENCES :

1. Physical Chemistry, 5th Ed., - Atkins, (ELBS) 1995
2. Introductory Quantum Chemistry – A.K.Chandra (Tata McGraw Hill) 1994.
3. Themodynamics - Rajaram and Kuriokose (East-West) 1986.
4. Statistical Thermodynamics, M. C. Gupta (Wiley eastern Ltd.) 1993.

THEORY-4:

Ch-2.4: MOLECULAR SYMMETRY AND SPECTROSCOPY-II 56Hours

UNIT – I : Symmetry and Group Theory 14 hrs

Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes, symmetry elements and symmetry operations, Schonflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. Reducible and irreducible representations. The Great Orthogonality theorem (without proof), character tables. The direct product. Applications of group theory - Molecular vibrations, group theoretical selection rules for electronic transitions, for infra red and Raman spectra. Hybrid orbitals and Molecular orbitals, transformation properties of atomic orbitals.

UNIT - II : 14 hrs

NMR of nuclei other than proton: ^{13}C chemical shift & factors affecting it Coupling constants. Decoupling-Noise decoupling & broad band decoupling. Off-resonance proton decoupling-some representative examples. ^{19}F & ^{31}P NMR- Predicting the spectra of simple inorganic compounds, NMR of paramagnetic complexes.

Electron Spin Resonance Spectroscopy: Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes.

NQR Spectroscopy: Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.

UNIT – III 14 hrs

Mössbauer spectroscopy: The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds(nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.

UV/Electronic Spectroscopy: Basic principles, Beer-Lambert law, molar absorptivity, energy levels, types of electronic transitions. Franck - Condon principles, ground and excited electronic states of diatomic molecules. Chromophores, auxochromes, electronic spectra of polyatomic molecules. Emission spectra, spectra of transition metal complexes, charge transfer spectra. Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting λ_{max} of organic compounds. Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.

Photoelectron spectroscopy: Basic principles, valence &core binding energies, shifts in energies due to chemical forces, Photoelectron spectra of simple molecules, Auger transitions, measurement techniques. Applications.

UNIT – IV 14 hrs

Mass Spectrometry :Basic principles, Instrumentation -Mass spectrometer, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations (fragmentation of organic compounds with respect to their structure determination) associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitrocompounds, amines & nitrogen heterocycles. Fragmentation patterns of carbohydrates, terpenoids, alkaloids, steroids, peptides & proteins-some representative examples, ion analysis, ion abundance, retro Diels-Alder fragmentation. Application in structure elucidiation and evaluation of heats of sublimation & ionization potential. Nitrogen rule. High resolution mass spectroscopy. 9 hrs

Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C NMR and mass spectroscopic techniques. Structural elucidation of organic molecules.

REFERENCES:

1. Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill)2001.
2. Organic Spectroscopy-3rd Ed.-W.Kemp(Pagrave Publishers, New York), 1991.
3. Spectrometric Identification of Organic Compounds - Silverstein,Bassler & Monnil l(Wiley)1981.
4. Applications of Absorption Spectroscopy of Organic Compounds-Dyer (Prentice Hall, NY)1965.
5. Spectroscopy of Organic Compounds-3rd Ed.-P.S.Kalsi (New Age, New Delhi) 2000.
6. E.A.V.Ebsworth, D.W.H.Ranklin and S.Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific, 1991.
7. R.S.Drago: Physical Methods for Chemists, Saunders College Publishing, 1992.
8. D.N.Satyanarayana: ElectronicAbsorption Spectroscopy and Related Techniques,
9. G.Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall, 2001
10. J. A. Iggo: NMR Spectroscopy in Inorganic Chemistry, Oxford University Press, 1999.
11. C.N.R.Rao and J.R. Ferraro: Spectroscopy in Inorganic Chemistry, Vol I&II(Academic)1970
12. Analytical Chemistry-Open Learning : Mass spectrometry.
13. Spectroscopic Methods in Organic Chemistry - Williams and Fleming, TMH.

Practicals:

1.Ch.Lab-2.1: Inorganic Chemistry -II
2.Ch.Lab-2.2: Organic Chemistry -II
3.Ch**.**Lab-2.3: Physical Chemistry-II
4.Ch.Lab-2.4: Applied Analysis -II

Note:Practicals are based on theory Papers exept Ch.Lab-1.4

THIRD SEMESTER SYLLABI OF M. Sc. PROGRAMMES IN CHEMISTRY

THEORY PAPERS:

THEORY-1:
Ch.-3.1: ORGANOMETALLIC CHEMISTRY 56Hrs

UNIT I: 14 hrs

Historical development- classification and nomenclature, bond energies and stability.
Transition metal alkyls and aryls- types, routes of synthesis, stability and decomposition pathways,. Nucleophilic and electrophilic cleavage of metal-carbon sigma bonded compounds. Alkane activation.
Transition metal to carbon multiple-bonded compounds- carbenes, carbynes, synthesis, nature of bond, agostic interactions, structural characteristics and reactivity. Transition metal hydrides – synthetic routes, structure and reactivity, synthetic applications.

Unit II: 14 hrs

Transition metal-carbon pi complexes: Preparative methods, nature of bonding, structural features of olefinic, acetylenic, allylic, butadiene, cyclobutadiene, η^5- cyclopentadienyl, η^6-benzene and other arenes, cycloheptatriene and cyclooctatetraene complexes.
Important reactions relating to nucleophilic and electrophilic attack on ligands.
Fluxional isomerism in olefin, allyl, dienyl and cyclopentadienyl complexes.
Isolobal concept.

Unit III: 14 hrs

Catalysis by organometallic compounds:16- and 18-electron rules, oxidative addition, insertion, deinsertion and reductive elimination reactions.
Homogeneous catalysis by organometallics- hydrogenation, hydrosilation, hydrocyanation and isomerization of olefins, immobilisation of homogeneous hydrogenation catalysts,
Hydrocarbonylation of olefins (oxo reaction–cobalt and rhodium oxo catalysts), carbonylation of alcohols- Monsanto acetic acid process. Polymerization of olefins and acetylenes: Ziegler-Natta catalyst systems. Fischer – Tropsch reaction , Water Gas Shift reactions.

Unit IV: 14 hrs

Organometallics in Organic Synthesis: Main group organometallics- preparation, properties and applications of organometallic compounds of Li, Mg, Hg, Zn, Cd and Sn. Synthetic applications of organo-transition metal compounds: organocuprates. Hydrozirconation, transmetallation reactions by organopalladiums and organonickels, carbonylation by metal carbonylates, decarbonylation, carbene complexes and metallacycles, arene complexes.

References:

1.J.P.Collman, L.S.hegedus, J.R.Norton and R.G.Finke: Principles and Applications of
2.Organotransition Metal Chemistry, University Science Books, 1987.
3.R.C.Mehrotra and A.Singh: Organometallic Chemistry, New Age International, 1999.
4.R.H.Crabtree:Organometallic Chemistry of Transition Metals, Wiley , 1999.
5.F.A.Cotton and G.Wilkinson : Advanced Inorganic Chemistry, Wiley, 1991.

THEORY-2:
Ch.-3.2: REACTION MECHANISMS AND NATURAL PRODUCTS 56Hrs

Unit-I 14 Hrs

Organic Name reactions: Reactions, Mechanisms and synthetic uses of the following: Stolbe condensation, Darzen condensation, Gattermann-Koch reaction, Cannizzaro reaction, Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith reaction, Stork Enamine reactions, Sharpless asymmetric epoxidation, Hofmann-Loffler-Freytag reaction, Suzuki coupling, Woodward and Prevost Hydroxylation, Bucherer reaction, Ullmann reaction. Wittig reaction-Mitsunobu reaction.

Unit-II 14 Hrs

Molecular rearrangements: Classification and general mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Intermolecular and Intramolecular migration, nature of migration and migratory aptitudes. Mechanism of Wagner-Meerwein, Dienone-Phenol, Pinacol-Pinacolone, Demaynov, Benzil-Benzilic acid, Fries, Wolff, Favorskii, Neber, Benzidine, Baeyer-Villiger, Beckmann, Lossen, Curtius, Schmidt, Stevens, Shapiro, Baker-Venkatraman and Amadori rearrangement.

Unit-III 14 Hrs

Natural Products:

Steroid: Introduction, Structure and synthesis of cholesterol. Estrone, progesterone, testosterone, androsterone and carticosterone, Biosynthesis of cholesterol.

Alkaloids: Introduction, Classification. Isolation and general methods of structural elucidation. Biological importance of alkaloids. Structure and synthesis of quinine, morphine, reserpine.

Terpenoids: Introduction, Classification and general methods of structural elucidation. Biological importance of terpenoids. Chemistry of pinene, camphor.

Anthocyanins: Introduction, general Nature of anthocyanin. Structure and synthesis of Anthocyanidins, Flavones and isoflavones.

Unit- IV 14 Hrs

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classifications of Pericyclic reactions. Woodward-Hoffmann correlation diagram and FMO approach.

Electrocyclic Reactions: Introduction, Con-rotatory & dis-rotatory Process, 4n&4n+2 ystems.

Cycloaddition reaction: Suprafacial and Antrafacial addition, 4n and 4n+2 systems.

Sigmatropic reactions: Suprafacial and Antrafacial shift of H, [1,3] & [1,5] -sigmatropic shifts. Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements.

References: -

1. O.L. Chapman, Organic Photochemistry. Vol I & II. Marcel Decker.
2. Francis A Carey and R. J. Sundberg, Advanced Organic Chemistry-Part A & (Plenum).
3. Mukherji Singh and Kapoor , Organic Chemistry, Vol 1-3, (Wiley Eastern, New Delhi)
4. Synthetic Organic Chemistry- G.R.Chatwal (Himalaya, Bombay), 1994.
5. Organic Reaction Mechanisms , V.K.Ahluwalia & R.K.Parashar (Narosa) 2006
6. Organic Chemistry, Vol I-II, I.L.Finar,(Longmann ELBS, London), 1973.
7. Advanced Organic Chemistry- Reaction Mechanisms, Reinhard Bruckner(Academic) 2005.
8. Pericyclic reactions, S.M Mukherji(The McMillan Bangalore), 1979.
9. Organic Reactions and their mechanisms- P.S.Kalsi (New Age, New Delhi), 1996.

THEORY-3:
Ch.-3.3:RADIATION AND PHOTOCHEMISTRY 56Hrs

UNIT - I : 14hrs

Nuclear structure and stability: Nuclear properties - nuclear forces, mass defect and binding energy. Nuclearstability-Liquid drop, shell and collective models. 3hrs

Radioactivity and Nuclear Decay - Decay modes of natural and artificial nuclides- Determination of half life, growth kinetics. Conditions of equilibrium. Theories of $\propto$, $\beta$and γ emissions. 3hrs.

Radiation Detection and Measurement: Experimental techniques in the assay of radioactive isotopes. Radiation Detectors-ionisation chambers, proportional and Geiger-Muller, scintillation and *semiconductor radiation detectors (NaI-Tl and Ge(Li), HPGe solid state detectors). Liquid scintillators* and multichannel analysers. 4 hrs.

Nuclear Reactions, Energy and Nuclear Power reactors - Nuclear fission and fusion.

Types of nuclear power reactors, basic features and components of a nuclear power reactor. An introduction to breeder reactors. 4 hrs.

UNIT – II: Nuclear Reactions and Radioisotopes: 14hrs

Radioisotopes: Definition of curie and related calculations. Production of radioisotopes and labelled compounds by bombardment. Radiochemical separation techniques- carriers, solvent extraction and ion-exchange methods. Szilard-Chalmer process. Physico-chemical and analytical applications-isotope dilution method, activation analysis, radiometric titration and C^{14} dating. Medical, agricultural and industrial applications of isotopes. 5hrs.

Radiation Chemistry: Difference between radiation and photochemistry. Radiation sources, units (LET, Rad, Roentgen and G-value), radiation dose and radiation chemical yield. Chemical Dosimetry-Fricke and ceric sulphate dosimeters. Radiation chemistry of water. A brief introduction to radiolysis of gases, liquids and solids. Techniques for study of transient species- Pulse radiolysis. Industrial applications of radiation chemistry (radiation synthesis, polymerization &, food irradiation) 6hrs.

Health and Safety Aspects: Biological effects of radiation, Hazards in radiochemical work. Radiation protection, permissible exposure doses. Radioactive waste management - 3hrs.

UNIT- III: Photochemistry 14hrs

Inroduction to photochemistry. Quantum yield and its determinations, experimental methods in photochemistry, Actinometry. Electronic energy states of atoms and molecules. -rules for transition between two energy states. Life time of excited electronic states. Frank- Condon principle.Absorption and emission spectra- effect of solute solvent interactions on electronic spectra-spectral shifts.Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants. Study of excited states by flash photolysis and laser beam experiments.

UNIT -IV: 14hrs

Photophysical pathways- Jablonski diagram, Radiationless transitions and selection rules. Flourescence and phosphorescence- theory and applications. Photochemical kinetics of unimolecular and bimolecular processes. Quenching-collisions in the gas phase, solution (Stern-Volmer equation) & by added substances. Photophysical Reactions-Types-Photo-dissociation, Isomerisation and other rearrangement reactions with specific examples. 12 hrs

A brief introduction to some current topics in photochemistry - Applications in synthesis, solar energy utilization and atmospheric chemistry. 2 hrs

REFERENCES:

1. Principles of Radiochemistry, Eds: Sood, Ramamoorthy & Reddy (IANCAS, BARC Mumbai)
2. Radiation Chemistry: An Overview, D.B. Naik and S. Dhanya (BARC, Mumbai)
3. Nuclear and Radiation Chemistry –Friedlander, Kennedy Macias & Miller (Wiley) 1981
4. Essentials of Nuclear Chemistry- H.J.Arnikar (Wiley Eastern) 1987.
5. An Introduction to Radiation Chemistry, Spinks and Woods (Wiley, New York) 1990
6. Fundamentals of Photochemistry – Rohatgi and Mukherje (New Age Bangalore) 2000.

THEORY-4:

Ch.-3.4: PRINCIPLAS OF ANALYTICAL CHEMISTRY 56Hrs

UNIT-I 14 hrs

Titration curves for strong acid-strong base, weak acid-strong base and weak base-strong acid titrations. Poly protic acids, poly equivalent bases. Determining the equivalence point-theory of acid-base indicator, colour change range of indicator, selection of proper indicator, indicator errors. Feasibility of acid-base titrations- magnitude of the equilibrium constant, effect of concentration. Typical applications of acid-base titrations Determination of nitrogen, sulphur, ammonium salts, nitrates and nitrites, carbonates and bicarbonates and organic functional groups like carboxylic acid, sulphonic acid, amine, ester, hydroxyl, carboxyl groups, air pollutants like SO_2.

Titrations in non-aqueous solvents –solvents for non-aqueous titrations, characteristics of amphiprotic solvents- Autoprotolysis, Dielectric constant. Meaning of pH. Aprotic solvents, choosing a solvent. Some selected solvents, titrants and standards. Titration curves, effect of water. Determining the equivalence point. Typical applications-determination of carboxylic acids, phenols and amines.

UNIT II 14 hrs

Redox titrations: Equilibrium constants for redox reactions - electrode potentials in equilibrium systems, calculation of equilibrium constants. Redox titration curves- formal potentials, derivation of titration curves. Factors affecting the shape of titration curves- concentration, completeness of reaction. Titration of mixtures- feasibility of redox titrations. Detections of end point -redox indicators, theory, specific and non specific indicators, choice of indicator, potentiometric end point detection. Sample preparation-prereduction and preoxidation. Karl Fischer reagent for water determination. Applications.

Gravimetry: Introduction to gravimetric analysis, precipitation methods, the colloidal state**,** Supersaturation and precipitate formation., purity of the precipitate: co-precipitation, post-precipitation, Conditions for precipitation, precipitation from homogeneous solution, washing the precipitate. Fractional precipitation, organic precipitants, volatilisation or evolution methods.

UNIT III: Basic concepts in electrochemical techniques 14 hrs

Electrochemical Cell: Components, conduction, reactions, liquid junctions, salt bridge representation. Faradaic and non-faradaic currents. Reversible and irreversible cells. **Electrode Potential:** Nature, measurement, sign convention, effect of concentration. Standard electrode potential, calculation limitations, **Cell Potential:** Thermodynamics, liquid junction potential, effect of current, ohmic potential, **Polarization:**Sources, overvoltage, concentration polarization, mechanism of mass transport, **Potentiometric methods:**Reference electrodes- calomel, silver/silver chloride and hydrogen electrodes, potentiometric titrations and applications, **Metallic Electrodes:** Electrodes of first, second & third kind, **Membrane Electrodes:**Classifications, properties, principle, design of ion selective electrodes, membrane potential, selectivity, crystalline liquid membrane and enzyme electrodes, **Glass Electrode**:Composition, hygroscopicity, asymmetry potential, acid and alkali errors, **Conductometric methods**: Definitions, conductance measurement, conductrometric titrations and applications

UNIT IV: Chromatographic Techniques 14hrs

Fundamentals of Chromatography : General description, definition, terms and parameter used in Chromatography, classification of Chromatographic methods, criteria for selection of stationery phase, and mobile phase, nature of adsorbents, factor influencing the adsorbent, Nature and type of mobile phase and stationery phase

Elution Chromatography: Van Deemter's equation, and its modern version, optimization of column performance, interrelationships-capacity factor, selectivity factor, column resolution, distribution constant and applications of conventional column Chromatography, advantages and limitations.

Thin Layer Chromatography (TLC): Definition, mechanism, efficiency of TL Plates. Methodology selection of stationery phase, and mobile phase, preparation of plates, spotting development, identification and detection, reproducibility of RF values, advantages and applications.

Gas Chromatography (GC): Principle, comparison of GSC and GLC, instrumentation column packed and tubular, study of detector-thermal conductivity, flame ionization, election capture and mass spectrometry, factors affecting separation, applications.

High pressure liquid Chromatography (HPLC): apparatus, pump, column packing, characteristics of liquid Chromatographic detector-UV, IR, refractometer and fluorescence detector, advantages and application.

REFERENCES:

1. Fundamentals of Analytical Chemistry –S.A. Skoog, West & Holler
2. Chemical Analysis - H.A. Laitenin, Mc Graw Hill (1960), 3. Analytical Chemistry- Larry G. Hargis.
4. Vogel's Text book of Quantitative Inorganic Analysis-Bessett,Denney, Jeffery &Mendham
5 Non-aqueous titrations-Walter Huber, Academic Press (1987), 6. Quantitative analysis- Kenner & Busch
6. Quantitative Analysis (5^{th} Edition) –R.A. Day and A. L. Underwood: P H I, 1988
7. Electroanalytical Chemistry –Vassos & Ewing, Wiley, N.Y., 1983;
8. Principles of Electroanalytical methods,Riley &.Tomlinson, Wiley, N.Y.,1987;
9. Principles of Instrumental Analysis- Skoog, 3^{rd} ed. Saunders College Pub. 1985;
10. Instrumental Methods of Chemical Analysis; B.K. Sharma, 19^{th} ed, Goel, 2000.

PRACTICALS:

Ch.Lab-3.1: INORGANIC CHEMISTRY PRACTICALS – III

A. Any five of the following experiments are to be carriedout:

1. Analysis of brass – Cu gravimetrically using ∝-Benzoinoxime and Zinc complexometrically.
2. Analysis Cu-Ni alloy .
3. Analysis of Stainless Steel – Insoluble residue by gravimetry, Ni gravimetrically using DMG, Fe volumetrically using Ce(IV) & Cr(III) volumetrically by persulphate oxidation.
4. Analysis of Type metal –Sn gravimetrically, Pb electrogravimetrically and Sb titrimetrically using $KBrO_3$
5. Quantitative analysis of the constituents & mixtures containing the following radicals
   (i) Cu(II) + Fe(II) - Cu gravimetrically as CuSCN and Fe using Ce(IV).
   (ii) Fe(II) + Ni(II) – Fe gravimetrically as Fe_2O_3 and Ni using EDTA.
   (iii) Fe(III) + Ca(II) - Fe gravimetrically as Fe_2O_3 and Ca using EDTA.
   (iv) Cr(III) + Fe(III) – Using EDTA by Kinetic masking method.
6. Analysis of chalcopyrites, magnetite and ilmenite.
7. Ion-exchange chromatography: Separation and determination of Mg^{2+}/Zn^{2+}, Zn^{2+}/Cd^{2+} & Cl^-/ Br^-.

B. Any five of the following experiments are to be carried out:

8. Determination of COD of a water sample
9. Determination of Phosphorus.
10. Determination of dissolved oxygen (DO) by Winkler's method
11. Determination of nitrate & nitrite in water samples and sea water.
12. Analysis of heavy metals in waste water, sea water (Pb, Hg etc. By spectrophotometry)
13. Determination of alkalinity of water samples
14. Determination of fluoride in drinking water by spectrophotometry and ion selective electrode
15. Determination of phosphates in detergents

REFERENCES :

1. A..I. Vogel : A Text book of Quantitative Inorganic Analysis, (ELBS), 1978.
2. APHA, AWWA and WPCF: Standard Method for the Examination of water and Waste Water (Washington DC),1989,
3. I. M. Kolthof and E.P. Sandell: Quantitative Chemical Analysis.McMillan,1980
4. I.Williams, Environmental Chemistry, Wiley, 2001
5. Lobinski and Marczenko, Comprehensive Analytical Chemistry, Vol.30, Elsevier,1996.

Ch.Lab-3.2: ORGANIC CHEMISTRY PRACTICALS - III

Quantitative determination of sugars, amino acids, phenols, carboxylic acids, amides, esters, aldehydes, ketones, urea by various methods. Determinations of acid and ester and acid and amide in mixtures of two.

Determination of functional groups like hydroxyl, vic-hydroxyl, enol, amino, amide.

Ch.Lab-3.3: PHYSICAL CHEMISTRY PRACTICALS – III

A. Electrochemistry: a. Conductometry (At least Three experiments to be carried out)

1. Determination of hydrolysis constants (aniline hydrochlride etc.).
2. Titration of a mixture of acetic acid, monochloro and trichloacetic acids with NaOH.
3. Determination of concentrations/amounts of sulphuric acid, acetic acid and copper sulphate by conductometric titration with sodium hydroxide.
4. Determination of oxalic acid by conductometric titration with sodium hydroxide.
5. Measurements of the conductance of a weak acid, HOAC and of the strong electrolytes NaOAc, HCl and NaCl and to calculate the ionisation constant of the acid.
6. Determination of pH and pK_a of a given weak acid at various dilutions.
7. Conductometric titration of the mixture of HCl and NH_4Cl.
8. Determination of activity coefficient of Zinc ions in 0.002M $ZnSO_4$.
9. Any other experiments of interest

b. Potentiometry (At least Three experiments are to be carried out)

1. Determination of pK values of maleic acid/malonic and phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
2. Determination of acidic and basic dissociation constants and isoelectric point an amino acid.
3. Determination of the potential of an electrochemical cell and mean ionic activity coefficient .
4. pH titration of (a) HCl versus NaOH, (b) $CuSO_4$ versus NaOH and (c) HOAC versus NaOH and (d) lead nitrate versus potassium chromate..
5. Determination of pK_a values of functional groups in amino acids using a pH meter.
6. Study of potential-pH diagrams.
7. Determination of activity coefficient of an electrolyte at different molalities.
8. Verification of Tafel equation of hydrogen evolution reaction.
9. Determination of pKa values of mono,di and tri-acid base.

B. Radiochemistry Experiments (At least Three experiments to be carried out)

1. Study of (a) Characteristic plateau, (b) Geometry effects and Statistics of G.M counter
2. Determination of (a) Dead time by double source method. (b) E_{max} of β - source (c) Back scattering of β and (d) β energy emitted by C- 14.
3. Verification of the inverse square law.
4. Determination of half life of radionuclides
5. Study of self adsorption of rays and determine the adsorption curve.
6. Preparation of Fricke and Ceric sulphate dosimeters & calculation of G-value&dose rate
7. Study of isotope dilution analysis.
8. Radio chemical Determination of I – 131 in sea water.

C. Photochemistry(Any Two experiments are to be carried out**)**

1. Irradiation of a reaction mixture and calculation of the quantum yield.
2. Determination of the quantum yield of chloride in the photohydrolysis of aqueous solution of monochloroacetic acid
3. Photochemical study of decomposition of hydrogen peroxide.
4. Photochemical study of Bleaching of dyes.

5. Photochemical reaction between threonine and ferrous sulphate.

D. Voltammetry & Polarography (Any Three experiments are to be carried out)

1. Determination of the half-wave potential of Cd(II), Cu(II)& Zn(II) ions in 0.1M solutions.
2. Determination of metal ions individually and in mixtures,
2. Determination of the formula and the stability constant of a lead oxalate.
3. Study of the polarogram of supporting electrolyte with and without dissolved oxygen,
5. Determination of Huckel β value of aromatic hydrocarbon reduction at dropping mercury electrode.

Ch.Lab-3.4: ANALYTICAL CHEMISTRY PRACTICALS – I

1. Determination of available K in soil,
2. Nephelometric determination of sulphate/phosphate.
3. Spectrophotometric determination of sulphur and phosphorus present in soil.
4. Determination of BOD of a water sample
5. Analysis of Na_2CO_3 in washing and baking soda by acid base titration
6. Enzymatic determination of glucose in blood by spectrophotometry.
7. Determination of blood urea and uric acid by spectrophotometry
8. Determination of iron in mustard seed by spectrophotometry
9. Extractive spectrophotometric determination of lead in leaf.
10. Determination of copper by potentiometric titration using EDTA.
11. Conductometric determination of total acidity of waste water.
12. Conductometric determination of chloride content of a sample of industrial effluent.
13. Analysis of $NaHCO_3$ in washing and baking soda by acid base titration
14. Amperometric titration

FOURTH SEMESTER SYLLABI OF M. Sc., PROGRAMMES IN CHEMISTRY

THEORY PAPERS:

THEORY-1:

Ch.-4.1: COORDINATION AND BIOINORGANIC CHEMISTRY 56Hrs

Unit I: 14 hrs

Spectral and Magnetic properties of complexes: Term symbols for d^n ions, spectroscopic ground states, selection rules, nature of spectral bands- band shapes, band intensities, band widths, spin-orbit coupling, vibrational structures.

Orgel diagrams, Tanabe-Sugano diagrams, interpretation of spectra of octahedral, distorted octahedral, tetrahedral and square planar complexes. Charge transfer bands – origin, types, and characteristics. Photochemistry of metal complexes- photosubstitution and photoredox reactions, ligand photoredox reactions, photoreactions and solar energy conversion.

Type of magnetic behaviour, orbital contribution, spin orbit coupling, measurement of magnetic susceptibility – Gouy and Faraday methods, diamagnetic corrections, ferro- and antiferromagnetic coupling, spin cross-over systems.

Unit II: 14 hrs

Reaction Mechanisms in Transition Metal Complexes**:** Energy profile of a reaction, inert and labile complexes, kinetics of octahedral substitution and mechanistic aspects. Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism and evidences in its favour. Anation reactions, reactions without M-L bond cleavage. Substitution reactions in square planar complexes, trans effect, mechanisms of substitution. Electron transfer reactions- inner sphere and outer sphere reactions, complimentary and non-complimentary reactions.

Unit III: 14 hrs

Metal ions in biological systems-essential and trace metals, ion transport across membranes, active transport of ions, ionophores.

Metalloproteins as enzymes- carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, catalases, peroxidases, cytochrome P 450, superoxide dismutase, copper oxidases, vitamin B_{12} coenzyme.

Unit IV: 14 hrs

Transport and storage of dioxygen- heme proteins, oxygen uptake, functions of haemoglobin, myoglobin, hemerythrin and hemocyanins, synthetic oxygen carriers.

Metal storage and transport – ferritin, transferrin and ceruloplasmin. Electron transfer proteins- cytochromes, iron-sulphur proteins. Biological nitrogen fixation, nitrogenase.

Metals in medicine- metal deficiency, metal toxicity, metal complexes as drugs

References:

1. D.N.Satyanarayana:Electronic absorption Spectroscopy and Related Techniques, OUP, 2001.
2. F.Basolo and R.G.Pearson: Inorganic Reaction Mechanisms, Wiley Eastern, 1979.
3. W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.
4. R.L.Dutta and A Syamal : Elements of Magnetochemistry, Affiliated east-West, 1993.
5. J.E Huheey, R.L.Keiter and A.L.Keiter: Inorganic Chemistry(4^{th} edn),Addison Wesley, 2000.
6. M.N.Hughes: Inorganic Chemistry of Biological Processes, (2^{nd} edn.) Wiley, 1988.
7. I.Bertini. H.B.Gray, S.J.Lippard and J.S.Valentine: Bioinorganic Chemistry, Viva Books, 1998.

THEORY-2:

Ch.-4.2: ORGANIC SYNTHETIC METHODS 56Hrs

Unit-I 14hrs

Reduction Reactions: Catalytic hydrogenation: Introduction, catalysts and solvents employed, reduction of functional groups, mechanisms and stereochemistry of catalytic hydrogenations, Hydrogenolysis, and homogeneous catalytic hydrogenation.

Mechanisms of reduction of conjugated system and carbonyl compounds, Bimolecular reductions of esters, Birch reduction, Reduction with hydrazine, and its derivative , Wolf-Kishner reduction and related reactions, Reduction with arene sulphonyl derivative of hydrazine, Reaction with diimide and related compounds.

Metal hydride reduction: Reduction with $LiAlH_4$ and $NaBH_4$, Stereo chemistry of reduction and other functional groups, Functional group transformation during reduction, Reduction with diborane and related reactions.

Unit-II 14hrs

Oxidation reactions: Introduction and different oxidative processes, Mechanism of oxidation reaction with chromium and manganese salts, peracids and peresters, periodic acid, Lead tetra acetate, Ozone, Osmium tetroxide and their synthetic importance in functional group transformation. **Halogenation:** Halogenation of olefins, carbonyl compounds, Benzyllic and Allylic halogenation, Dehalogenation reactions. Dehalogenation with S, Se, Pt, Pd, Ni.

Unit-III 14hrs

Synthetic Design: Carbon skeleton frame work, Classification of carbon-carbon single bond and double bond forming reaction and their use in carbon skeleton ring formation. Ring forming and ring cleaving reactions, use of Thorpe condensation, Carbene insertion reaction, Friedel-Crafts reaction, 1,3-dipolar addition and Ene reaction in ring formation, Oxidative cleavage of rings and Retro Diel's-Alder reactions.

Planning of organic synthesis: Selection of starting materials and key intermediates during the synthesis. Synthesis of Cubane and Iswarane. Use of Robinson annulation, Dickmann cyclisation, Arndt-Eistert synthesis and Diel's- Alder reaction in organic synthesis.

Functionality: Synthesis of 6- and 7- methoxy tetralones, biotin and penicillin-V with special reference to the introduction of functional groups. Stereo chemical consideration and stereo selectivity during organic synthesis.

Unit-IV 14hrs

General introduction to disconnection approach. Basic principles and technologies used in disconnection approach. Synthons and synthetic equivalents. Interconversion of functional groups. One group C_X and two group. C_X disconnections.

Protecting groups: Principle of protection of hydroxyl amino carboxylic and carbonyl groups.

Retrosynthetic analysis: Analysis of alcohols, carbonyl compounds cyclic and acyclic alkanes, benzocaine, p-methoxyacetophenone, acetonecyanohydrin, 2-methyl-6-methoxy-indole-3-aceticacid, 6-methylquinoline & 1-phenyl-4-p-methoxyphenyl-1,3-butadiene

References :-

1. Modern Organic Reactions- H.O.House.
2. Organic Synthesis- R.E.Ireland (Prentice Hall India), 1969.
3. Art in Organic Synthesis- Anand, Bindra & Ranganath-(Wiley New Delhi), 1970.
4. Organic Synthesis a Disconnection Approach- Stuart
5. Advanced Organic Chemistry-IV-Ed. Part A &B-F.J.Carrey & R.J.Sundberg(Kluwer) 2001.
6. Modern Methods of Organic Synthesis-N.Carruthers(Cambridge University), 1996.

THEORY-3:

Ch.-4.3: CHEMICAL DYNAMICS AND CATALYSIS 56Hrs

UNIT -I : 14Hrs

Principles of Reactivity: An overview of basic kinetic concepts and analysis of kinetic results - rates of simple and composite chemical reactions (simultaneous and consecutive), steady-state treatment, rds, microscopic reversibility, empirical rate equations - methods of determining rate laws. - Statistical treatment of rates – Transition state theory and its limitations and extensions. Applications to reactions in solution. Activation parameters from experimental results, mechanistic significance and their uses General approaches in elucidating reaction mechanism - kinetic and thermodynamic control of reactions. Reactivity - selectivity principles (Hammond's postulate & Curtin-Hammet principle). 9 hrs

Complex reactions–Mechanisms of some inorganic and organic reactions- comparison of hydrogen - halogen reactions, formation and decomposition of phosgene, decomposition of N_2O_5, ozone, acetaldehyde and ethane, Nucleophillic and electrophillic substitution reactions. 5 hrs.

UNIT -II : 14Hrs

Potential energy surfaces – Features & construction of them. Theoretical calculation of Ea. Dynamics of unimolecular reactions-Lindemann, Hinshelwood, RRK & RRKM theories. 5 hrs.

Fast Reaction Techniques – Flow, flash photolysis, relaxation and nuclear magnetic resonance methods. A brief molecular beam studies of reactive collision/scattering-stripping and rebound mechanisms, state-to-state kinetics and spectroscopy of transient species 6 hrs.

Theory of kinetic isotope effects - Primary, secondary and solvent kinetic isotope effects. Tunneling effect. Isotope effects with heavier atoms. 3 hrs.

UNIT -III : 14Hrs

Substituent Effects on Reactivity: Inductive effect, electromeric effect, substitutions and the energy of activation. Hammett & Taft equations, Deviations from Hammett equation. Dual-parameter correlations- σ_1- and σ_R- scales: Swain-Scott & Edward equations, Winstein Grunwald relationship, Isokinetic relationship, significance of isokinetic temperature, exner criterion. LFERs. 6 hrs

Solvation and Solvent Effects: Cage effect, effects of ionic strength, dielectric constant and solvation on rates of reactions (ion-ion, ion-dipole& dipole-dipole reactions). 3 hrs

Homogeneous catalysis: Electronic and structural effects on acidity and basicity. Hard and soft acids and bases. Acidity functions - Hammett acidity function, Zucker–Hammett hypothesis. Bunnett hypothesis. Industrial catalysts: Catalyst carrier, promoter, inhibitor & catalyst poison. 5 hrs

UNIT- IV: **14Hrs**

Reactions at Surfaces: Structures of solid surfaces & adsorbed layers. Mechanisms of surface reactions- kinetic effects of surface heterogeneity & interactions – surface inhibition and activation energies –reactions between two adsorbed molecules – surface exchange reactions – Transition state theory of surface reactions – unimolecular and bimolecular reactions. Comparison of homogeneous & heterogeneous reaction rates. Liquid-air, liquid-liquid & solid-liquid interfaces. **8 hrs**

Micelles: Surface active agents-micellisation, hydrophobic interactions, critical micellar concentration (CMC), factors affecting the CMC of surfactants. Micellar catalysis**. 3 hrs**

Pharmaco kinetics: Pharma concentration time curve, protein binding and drugs, drug dissolution rate, pharmacokinetics applied to one-component open model (calculation of elimination rate constant & metabolism constant**). 3 hrs**

REFERENCES :

1. Physical Chemistry, 5th ed., - Atkins (ELBS) 1995
2. Chemical Kinetics - K.J.Laidler (Pearson Education) 1987.
3. The Physical Basis of Organic Chemistry, H.Maskill, Oxford University Press.
4. Physical Organic Chemistry, N.S.Isaacs, ELBS/Longman.
5. Catalysis - J.C. Kuriacose (Macmillan India Ltd.) 1991.
6. Micelles, Theoretical and applied aspects, V.Moroi, Plenum.

PRACTICALS:

Ch.Lab-4.1: INORGANIC CHEMISTRY PRACTICALS - IV

1. Colorimetric determination of Ti(IV) and Zr(IV)
2. Simultaneous colorimetric determination of two metal ions – Mn and Cr.
3. Flame photometric determination of Na, K, Li and Ca individually and in mixtures.
4. Electrogravimetric determination of (a) Cu-Ni alloy and (b) Pb in Type Metal.
5. Solvent extraction of Ni(II) and UO_2(II).
6. Preparation of any three of the following complexes, checking the purity of the prepared samples by chemicals analysis, structural study of the prepared complexes using conductance and magnetic susceptibility measurements, recording the electronic and infrared spectra:
   i) Chloropentamminecobalt(III) chloride, ii) Hexamminecobalt(III)chloride.
   iii) Potassium trisoxalatoferrate(III) and iv) Potassium hexathiocyanatochromate(III)
   v) $K_3Cr(OX)_3.3H_2O$ vi) $Cu(tu)_3Cl$ vii)$Zn(tu)_3OSO_3$
7. Determination of composition of complexes:
   a) Job's method: Fe-phenanthroline complex
   b) Mole ratio method: Zr-Alizarin red S complex,
   c) Slope ratio method: Cu ethylenediamine complex,
   d)Limiting logarithmic method:Uranyl-sulphosalicyclic acid complex.
8. Determination of stability constants
   a) Turner Anderson method : Fe-Tiron system,
   b) Bejrrums's method : Cu – sulphosalicyclic acid system,
   c) Polarographic method :Cu-glycinate or Pb -oxalate system.

References:

1. J. Rose, Physicochemical Experiments
2.Vogel's Text Book of Quantitative Chemical Analysis(5th Ed), G.H.Jeffrey, J.Bassette, J.Mendham and R.C.Denny, Longman, 1999.

Ch.Lab-4.2: ORGANIC CHEMISTRY PRACTICALS - IV

Multi Step Organic Synthesis

Ethyl resorcinol from Resorcinol, 3-Bromo-4-methyl benzaldehyde from p-Toludine, ε-Caprolactam from cyclohexanone, p-Amionobenzoic acid from p-Nitrotoludine, s-Tribromobenzene from aniline, o-hydroxy acetophenone from phenol, Benzanilide from Benzophenone, Benzylic acid from Benzoin, Benzopinacolone from Benzophenone, p-Chlorotoluine from p-Toludine, 2,5-Dihydroxy acetophenone from Hydroquinone, 2,4-Dinitrophenylhydrazine from Chlorobenzene, m-Nitrobenzoic acid from Benzoic acid, 2,4-Dinitrophenol from Chlorobenzene, o-Aminobenzoic acid from Phthalic anhydride, 2-Carbethoxycyclopentanone from Adipic acid, α-Acetylamino cinnamic acid from Glycine, p-Aminoazobenzene from Aniline.

Separation of components from mixture of organic compounds by fractional crystallization, fractional distillation, adsorption, Paper and TLC. Their purification and characterization.

Ch.Lab-4.3: PHYSICAL CHEMISTRY PRACTICALS - IV

A. Kinetics and Catalysis (Any Five Experiments are to be carried out)

Determination of reaction order and activation parameters, study of acidity/salt/solvent/, catalytic effects on reaction rates of any FIVE of the reactions listed below.

1. Acid catalysed hydrolysis of methyl acetate.
2. Saponification of ethyl acetate by conductivity method.
3. Decomposition of benzenediazonium chloride.
4. Reaction betweem potassium persulphate and potassium iodide (including the study of salt effect and catalysis by Ag^{+}, Fe^{2+} and Cu^{2+} ions).
5. Decomposition of diacetone alcohol by NaOH & Hydrolysis of t-Butylchloride.
6. (i) Reaction between iodine and acetone and (ii) iodination of aniline.
7. Reaction between hydrogen peroxide and HI.
8. Decomposition of H_2O_2 (including the study of catalytic effect).
9. Reaction between Chromic acid and oxalic acid. 11. Iodine clock reactions.
10. Reduction of aqueous solution of ferric chloride by stannous chloride.

B. Polymer Chemistry (Any Two experiments are to be carried out)

1. Determination of molecular weight and size parameters of polymers by viscometry.
2. Determination of sequences in polyvinylalcohol by viscometry.
3. Determination of molecular weight of a polymer by turbidimetry.
4. Preparation of Polymethylmethacrylate by suspension polymerization / polystyrene by free radical polymerization / Nylon by interfacial polymerization / Polyacrylamide by solution polymerisation method / polyvinylalcohol from polyvinylacetate / Phenol formaldehyde/ urea formaldehyde resins / thin films of polymers.

C. Thermodynamics Experiments (Any Five experiments to be carried out)

1. Determination of activities of an electrolyte and non – electrolyte by cryoscopy.
2. Study of association of benzoic acid in benzene.
3. Determination of partial molar volumes of (a) Salts – water and (b) alcohol – water (methanol & ethanol) systems by density method.
4. Study of complex formation between mercury and potassium halides by cryoscopy.
5. Determination of specific heat of liquids and solutions by calorimetry.
6. Determination of stepwise neutralisation of acids.
7. Study of phase diagram of a ternary aqueous system of potassium chloride and water.
8. Study of phase diagram of a ternary system of benzene – acetic acid – water or DMSO- water – benzene or ethanol – benzene – water etc.
9. Determination of heat of solution of KNO_3 in water, integral heat of dilution of H_2SO_4 and heat of ionization of acetic acid and ammonium hydroxide calorimetrically.
10. Cryoscopic and ebullioscopic analysis of the given mixture of urea and glucose.
11. Determination of vant Hoff's factor for benzoic and acetic acid mixtures in benzene.
12. Determination cryoscopically the pH value of 0.5 M malonic acid in water.
13. Determination of heat of neutralisation of two acids and hence their relative strength.
14. Study of adsorption of picric acid on charcoal using a calorimeter.

D. Spectrophotometry (Any Two experiments are to be carried out)

1. Determination of pKa values of indicators. 2. Determination of Hammett's acidity function.
2. Spectroscopic investigation of partition coefficient of iodine between H_2O and $CHCl_3$.
3. Study of the effect of ionic strength on the pH of the given acid with the help of indicators using buffer solution by colorimetric method.

Ch.Lab-4.4: ANALYTICAL CHEMISTRY PRACTICALS – II

1. Analysis of saccharin in tablets by argentometric titration.
2. Determination of mercury in algaecide by EDTA titration.
3. Determination of CaO in the given cement solution
4. Determination of sulphate in ground water samples by Spectrophotometric method
5. Determination of Sodium content in the blood sample.

6.Determination of CO_2 in the sewage water sample
7. Determination of potassium in soil by flame photometry.
8. Polarographic determination of Cd and zinc in solutions individually and in a mixture
9.Determination of Total Nitrogen in the soil sample by Kjedhal's method.
10. Nephelometric determination of phosphate in domestic waste water.
11. Analysis of lead in industrial effluents by spectrophotometry
12. Analysis of copper in bronze alloy by iodometric titration

REFERENCES:

1.A Text Book of Quantitative Inorganic Analysis – A.I. Vogel
2.Vogel's Text Book of Quantitative Inorganic Analysis,Basset, Denney, Jeffery&Mendham
3.Colorimetric Determination of Traces of Metals – E. B. Sandell.

INTERDISCIPLENARY ELECTIVES

Ch.EL-1A:SOLID STATE CHEMISTRY **28Hrs**

UNIT –I: 14 hrs

Crystal Defects and Non-Stoichiometry: Perfect and imperfect crystals, intrinsic and extrinsic defects- point, line and plane defects.Vacancy, Schottky and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects – Structures of UO_2, FeO and TiO. . 5 hrs

Solid State Reactions: General Principles, Wagner's theory. Order - disorder transitions in solids-Bragg- William's theory Mechanism of diffusion , Kirkendall effect. 4 hrs

Preparative Methods: Ceramic, sol-gel, precursor and chemical vapour deposition (CVD) methods. Nucleation & crystal growth techniques-pulling, zoning, flame fusion & skull melting. Basic methods of preparation of thin films . 5 hrs

UNIT – II : 14 Hrs

Electronic Properties and Band Theory: Free electron theory to band theory of solids, electrical conductivity, Hall effect. Metals, Insulators and Semiconductors. Intrinsic and extrinsic semiconductors, hopping semiconductors. Metal – semiconductor and p-n junctions. 5 hrs

Insulators-Dielectric, ferroelectric, pyroelectric & piezoelectric properties & their applications. 4 hrs

Magnetic properties: Classification of magnetic materials – dia, para, ferro, ferri, antiferro & antiferri magnetic types Langevin diamagnetism. Selected magnetic materials such as spinels & garnets. 5 hrs

REFERENCES :

1. D. K. Chakrabarty, Solid state chemistry (New Age) 1996.
2. H.V.Keer, Principles of the solid state (Wiley Eastern) 1993.
3. A.R.West, Solid state chemistry and its applications (Wiley) 1984.
4. L.Smart and E. Moore, Solid State Chemistry –An Introduction (Chapman &Hall)1992.
5. L. Azaroff, An Introduction to Solids (Mc Graw Hill).
6. M. M. Woolfson, An Introduction to X-ray Crystallography, Vikas, New Delhi (1980).
7. C. Kittel, Introduction to Solid State Physics, Wiley Eastern Ltd., New Delhi (1987)
8 V. Raghavan, Material science and Engineering (3rd Ed), (Prentice Hall India)1993.
9. Thermotropic Liquid Crystals, Ed. G.W. Gray, Wiley.
10. S.Chandrasekhar, Liquid Crystals, Cambridge University Press (2nd ed), 1994.

Ch.EL-1B:ENVIRONMENTAL CHEMISTRY 28Hrs

UNIT IV: Water Pollution and Analysis 14 hrs

Water resources, origin of waste water, types of water pollutions, their sources and effects. Chemical analysis for water pollution control- objectives of analysis, parameters of analysis, sample collection and preservation. Environmental/public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphates, and different forms of nitrogen in natural and waste/polluted waters. Heavy metal pollution –public health significance of Pb, Cd, Cr, Hg, As, Cu, Zn, Mn. General survey of the instrumental techniques for the analysis of heavy metals in aquatic systems. Organic loadings-significance and measurement of DO, BOD, COD, TOD and TOC. Phenols, pesticides, surfactants, tannin and lignin as water pollutants and their determination.

UNIT II : Air Pollution and Analysis 14 hrs

Classification and properties of air pollutants. Emission sources, major emissions from global sources. Behaviour and fate of air pollutants –wet precipitation, dry deposition, interaction at the earth's surface, chemical reactions in the atmosphere, photochemical smog. Effects of air pollution on human health, vegetation and materials, Air pollution sampling and measurement- ambient air sampling, collection of gaseous and particulate air pollutants. Analysis of air pollutants. SO_2 –ambient air measurements, stack gas measurement NOx –Griess-Saltzmann and Jacob-Hocheiser methods, chemiluminescent techniques.CO-NDIR, amperometric, FID & catalytic oxidation methods. Oxidants & ozone-colorimetric, coulometric & chemiluminescent methods. **Hydrocarbons**-total and individual hydrocarbons by chromatographic methods. Particulates optical & mass measurement methods.

REFERENCES:

1. Environmental Chemistry – Manahan, S.E, Lewis Pub., 4th ed., Columbia (1990)
2. Air Pollution – B.G. Liptak;
3. Water Pollution – B.G. Liptak
4. Chemistry for Environmental Engineering–Sawyer and McCarty, 3rd ed., McGraw Hill1978
5. Environmental Chemistry – A.K. De;
6. Environmental Pollution Control and Engineering–C.S.Rao,Wiley-Eastern, New Delhi,1991;
7. Standard Methods for examination of water waster water–15th ed., Ed.Greenberg, Connors and Jenkins, APHA (1981);
8. Technical Methods of Analysis – R.C. Griffin
9. Instrumental Analysis for Water Pollution Control–M.Nancy, Ann Arbor, Michigan 1971

DAVANGERE UNIVERSITY

Department of Chemistry

M.Sc Course Pattern and Scheme of Examination under CBCS approved by PG-BOS in Chemistry.

Quation Paper Pattern for Chemistry

A.THEORY PAPERS:

The Syllabus of each paper shall be grouped into units of 14 teaching hours Question Papers in all the four semesters shall consist of Parts A and B. Part A shall contain twelve (12) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (3 questions per unit). Ten (10) questions are to be answered. Part B shall contain eight (8) brief and/or long answer questions carrying 11 marks each drawn from all the four units of the syllabus (2 questions per unit). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Five (5) out of eight (8) questions are to be answered

B.ELECTIVE PAPERS:

The Question Papers shall consist of Parts A and B. Part A shall contain six (6) very short answer objective type questions carrying 2 marks. Five (5) questions are to be answered.

Part B shall contain Five (5) brief and/or long answer questions carrying 10 marks each drawn from the two units of the syllabus (Atleast 2 questions per unit). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division (3+3+4 or 5+5). Three (3) out of Five (5) questions are to be answered.