VIJAYANAGARA SRI KRISHNADEVARAYA UNIVERSITY, BELLARY

CHEMISTRY (PG)

(2013-14)

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Credit Based, Choice Based, Continuous Assessment Patterned Semester Scheme.

The Board has framed and approved the Syllabus / Scheme of examination of Choice Based Credit Based System (CBCS) and recommended for implementation from 2013-2014. The following are the core papers and scheme of examination proposed by the Board.

1. M.Sc, Degree in Chemistry I & II Semester
2. M.Sc, Degree in Chemistry – III and IV Semester.

The pattern of matrix for two year Master's Degree Program in Chemistry:

No	COURSES	I SEM			II SEM			III SEM			IV SEM			TOTAL		
		C	P	M	C	P	M	C	P	M	C	P	M	C	P	M
1.	HARD CORE (Theory)	12	3	300	12	3	300	12	3	300	12	3	300	48	16	1200
2	HARD CORE(Practicals)	6	3	150	6	3	150	4	2	100	4	2	100	20	10	500
2.	SOFT CORE	4	1	100	4	1	100	4	1	100	4	1	100	16	4	400
3.	OPEN ELECTIVE	-	-	-	2*	1	50	2*	1	50	-	-	-	04	2	100
	TOTAL	**22**	**5**	**550**	**24**	**6**	**600**	**22**	**6**	**550**	**20**	**5**	**500**	**88**	**22**	**2200**

***The M.Sc. Chemistry students have to choose open elective papers from other disciplines**

COURSE STRUCTURE AND SCHEME OF EXAMINATION

M.Sc. DEGREE IN CHEMISTRY
FIRST SEMESTER

THEORY

Hard Core Papers	Paper Title	Contact Hours/ Week & Credits	Total Marks/Paper	Assessment Weightage		Semester End Exam Duration(hrs) & Assessment Weightage
				I test	II test	
CHI HCT:1.1	Concepts and Models of Inorganic Chemistry	4h &4	100	15%	15%	3h & 70%
CHO HCT:1.2	Theoretical Organic Chemistry	4h &4	100	15%	15%	3h & 70%
CHP HCT:1.3	Chemical Thermodynamics and Chemical Kinetics	4h &4	100	15%	15%	3h & 70%
Soft Core Papers Soft Core-I (For Chemistry Students Only)						
CSA SCT:1.4 OR CSM SCT:1.5	Analytical Chemistry - I	4h &4	100	15%	15%	3h & 70%
	Mathematics & Computer for Chemists	4h &4	100	15%	15%	3h & 70%

PRACTICALS

Hard Core Papers	Paper Title	Contact Hours/ Week & Credits	Total Marks/Paper	Assessment Weightage		Semester End Exam Duration(hrs) & Assessment Weightage
				I test	II test	
CHI HCP:1.6	Inorganic Chemistry	4h &2	50	15%	15%	4h & 70%
CHO HCP:1.7	Organic Chemistry (preparations)	4h &2	50	15%	15%	4h & 70%
CHP HCP: 1.8	Physical Chemistry	4h &2	50	15%	15%	4h & 70%

Note:

1. All hard core papers are **compulsory** for all the students.
2. The students of chemistry have to select **one** of the two soft core papers.
3. Students of both chemistry & non-chemistry, when register for additional credits, can opt for more than one soft core papers. However a minimum of ten students have to register for additional credits for operationalization of such a paper.
4. Open elective / cross border-papers are for other than chemistry students. Students have to opt one of the two open elective papers. However for operationlization of such paper, a minimum of **ten** students are required to opt such a paper

M.Sc. DEGREE IN CHEMISTRY
SECOND SEMESTER

THEORY

Hard Core Papers	Paper Title	Contact Hours/ Week & Credits	Total Marks/ Paper	Assessment Weightage		Semester End Exam Duration(hrs) & Assessment Weightage
				I test	II test	
CHS HCT:2.1	Co-ordination Chemistry	4h &4	100	15%	15%	3h & 70%
CHO HCT:2.2	Heterocyclic Chemistry, Natural Products & reagents	4h &4	100	15%	15%	3h & 70%
CHP HCT:2.3	Electro-,Quantum-& Photo Chemistry	4h &4	100	15%	15%	3h & 70%
Soft Core Papers, Soft Core-II (For Chemistry Students Only)						
CSA SCT:2.4 OR CSB SCT:2.5	Analytical Chemistry – II	4h &4	100	15%	15%	3h & 70%
	Selected Topics in Chemistry-I	4h &4	100	15%	15%	3h & 70%

PRACTICALS

Hard Core Papers	Paper Title	Contact Hours/ Week & Credits	Total Marks/Paper	Assessment Weightage		Semester End Exam Duration(hrs) & Assessment Weightage
				I test	II test	
CHI HCP:2.6	Inorganic Chemistry	4h &2	50	15%	15%	4h & 70%
CHO HCP:2.7	Organic Chemistry (Qualitative Analysis)	4h &2	50	15%	15%	4h & 70%
CHP HCP: 2.8	Physical Chemistry	4h &2	50	15%	15%	4h & 70%
OPEN ELECTIVE/ CROSS BORDER PAPER-I (FOR NON – CHEMISTRY STUDENTS ONLY) **THEORY**						
OET SCT:2.1 OR OET SCT:2.2	Environmental Chemistry	2h &2	50	15%	15%	2h & 70%
	Inorganic & Physical Chemistry	2h &2	50	15%	15%	2h & 70%

Note:

1. All hard core papers are **compulsory** for all the students.
2. The students of chemistry have to select **one** of the two soft core papers.
3. Students of both chemistry & non-chemistry, when register for additional credits, can opt for more than one soft core papers. However a minimum of ten students have to register for additional credits for operationalization of such a paper.
4. Open elective / cross border-papers are for other than chemistry students. Students have to opt one of the two open
   Elective papers. However for operationlization of such paper, a minimum of **ten** students are required to opt such a paper
5. The students have to choose Open Elective paper from the other departments.

M.Sc, DEGREE IN CHEMISTRY
THIRD SEMESTER

THEORY

Hard Core Papers	Paper Title	Contact Hours/ Week & Credits	Total Marks/Paper	Assessment Weightage		Semester End Exam Duration(hrs) & Assessment Weightage
				I test	II test	
CHI HCT:3.1	Spectroscopy-I	4h &4	100	15%	15%	3h & 70%
CHS_2 HCT:3.2	Nuclear Chemistry and Materials Science	4h &4	100	15%	15%	3h & 70%
CHP HCT:3.3	Advanced Physical Chemistry	4h &4	100	15%	15%	3h & 70%
Soft Core Papers Soft Core-III (For chemistry students only)						
CSA SCT:3.4	Applied Analysis	4h &4	100	15%	15%	3h & 70%
CSE SCT:3.5	Environmental and Biochemical Analysis	4h &4	100	15%	15%	3h & 70%

PRACTICALS

Hard Core Papers	Paper Title	Contact Hours/ Week & Credits	Total Marks/Paper	Assessment Weightage		Semester End Exam Duration(hrs) & Assessment Weightage
				I test	II test	
CHI HCP:3.6	Inorganic Chemistry	4h &2	100	15%	15%	4h & 70%
CHI HCP:3.7	Organic Chemistry (Estimations)	4h &2	100	15%	15%	4h & 70%
OPEN ELECTIVE/CROSS BORDER PAPER-II(FOR NON – CHEMISTRY STUDENTS ONLY) THEORY						
0ET SCT:3.8 OR OET SCT:3.9	Organic & Analytical Chemistry	2h &2	50	15%	15%	2h & 70%
	Quality Control Assurance & Chromatographic Techniques	2h &2	50	15%	15%	2h & 70%

Note:

1. All hard core papers are compulsory for all the Chemistry students
2. The students of chemistry have to select **one** of the two soft core papers.
3. A minimum of **ten** students have to opt for soft core papers for operationalization.
4. The students have to choose Open Elective paper from the other departments.

M. Sc. DEGREE IN CHEMISTRY
FOURTH SEMESTER

THEORY

Hard Core Papers	Paper Title	Contact Hours/ Week & Credits	Total Marks/Paper	Assessment Weightage		Semester End Exam Duration(hrs) & Assessment Weightage
				I test	II test	
CHO HCT:4.1	Advanced Organic Chemistry (Hormones, Stereo selective synthesis, Photochemistry, Heterocyclic Chemistry)	4h &4	100	15%	15%	3h & 70%
CHI HCT:4.2	Advanced Inorganic Chemistry	4h &4	100	15%	15%	3h & 70%
CHS HCT:4.3	Spectroscopy-II	4h &4	100	15%	15%	3h & 70%
CHP HCP:4.6	Project Work	8h &4	100	15%	15%	Project viva & evaluation 70%
Soft Core Papers Soft Core – IV						
CHP SCT: 4.4	Polymer Science and Technology	4h &4	100	15%	15%	3h & 70%
CHA SCT: 4.5	Advanced Topics in Chemistry	4h &4	100	15%	15%	3h & 70%

Note:

1. All hard core papers are compulsory for all the Chemistry students
2. The students of chemistry have to select **one** of the two soft core papers.
3. A minimum of **ten** students have to opt for soft core papers for operationalization.

Theory question paper format for CBCS Semester Examinations:

Part – A (Compulsory)

Q.1 Ten sub questions carry one mark each. **Total 10 marks**.

Part – B

Will consist of four questions, one from each unit of **15 marks**. Each question will have sub-divisions a, b, & c with an internal choice for only sub-section c. **Marks 15X4=60**

Time Duration: 3 Hrs **Total Marks=70**

Question paper format for Open Elective:

Part –A (Compulsory)

Q-1. Five sub-questions carry one mark each. **Total 05 marks**.

Part –B

Will consist of two questions one from each unit of **15 marks**. Each question will have sub-divisions a, b, & c with an internal choice for only sub-section c.

Time Duration: 1 ½ Hrs **Marks 15X2=30**

***CHP HCP: 4.6- Project work:**

The project work may include in plant training* in an Industry/Short term work in the department/other educational institutes/R&D organization/Data mining/Review of current literature/Theoretical methods/Computer applications. Experimental work may involve studies on Synthesis/Measurements, Study of properties/Characterization by physico-chemical methods/activities for reported/unreported research or any suitable combination thereof.
Incase of the student who would work outside the campus, the supervising staff members may visit to the work place at least once during the period and may be eligible for TA/DA as per the University rules. The other general academic regulations will be same as laid by University.

Evaluation of project work:

C1- 15%: Literature survey and submission of synoptic note
C2- 15%: Oral presentation of the project work under study.
C3- 70%: 50 marks for Project report
20 marks for Viva-voce examination.

M.Sc. DEGREE IN CHEMISTRY
FIRST SEMESTER

THEORY

CHI HCT:1.1 Concepts and Models of Inorganic Chemistry:

56 Hrs.

UNIT-I

Review of periodic properties- atomic size, ionization potential, electron affinity and electro negativity.

Ionic Bond:

Ionic bond-properties of ionic compounds, ionic radii, factors affecting ionic radii, radius ratio rules, types and structures of simple ionic compounds, lattice energy, Born-Lande equation, Born-Haber cycle-applications, size effects, polarizing power and polarizability of ions, Fajjan's rule, covalent character in ionic compounds, solutions of ionic solids and hydration energy.

Covalent Bond and Metallic Bond:

VBT approach, VSEPR-shapes of molecules, concepts of resonance and hybridization, Energetics of hybridization, partial ionic character, covalent coordinate and multicentre bonding, M.O theory-LCAO approach, σ, δ and Π molecular orbits. M.O treatment of homo nuclear and hetero nuclear diatomic molecules, Bond order – delocalized Π - bonding systems, Ex: CO_3^{2-}, NO_3^-, SO_3. Metallic bonding – electron sea model, VBT.

[14 hrs]

UNIT-II

Chemistry of Transition Metals:

Coordination numbers, factors affecting coordination numbers, stereochemistry of coordination compounds. Catalytic properties, non-stoichiometry, metal-metal bonding and cluster compounds, stability of oxidation states.

Chemistry of lanthanides and actinides-trends in physical and chemical properties, stereochemistry, magnetic and spectral behavior, synthesis and separation of trans-uranium elements, super heavy elements.

[14 hrs]

UNIT-III

Chemistry of S and P-Block Elements:

Alkali metals, alkaline earth metals and their complexes, crown ethers, oxides of alkali metals. Synthesis ,properties and structure of boron hydrides, boranes, borazines, boron-phosphorus and boron-arsenic compounds. Oxides and oxy acids of nitrogen, phosphorus, sulphur and halogens. Interhalogen compounds and noble gas compounds, silicates and zeolites.

[14 hrs]

UNIT-IV

Acid – Base Concept:

Introduction different definitions, types of reactions, solvent systems and leveling effect. Generalized acid-base concept-basicity of metal oxides, hydration and hydrolysis. Measurement of acid – base strengths. Steric affects-back strain, front strain and internal strain. Solution effects with respective to liquid ammonia, anhydrous sulphuric acid, acetic acid and liquid sulphur dioxide, acetic acid, HF, N_2O_4 and molten salts. HSAB-classification & strength of hardness and softness. Irving-William's series. Theoretical bases of hardness and softness.

[14 hrs]

REFERENCES

1. Basic Inorganic Chemistry – 3rd edition, F.A Cotton, G.Wilkinson and P.L.Gaw, John wiley and sons (2002).
2. Inorganic chemistry – James E Huheey, Harper and Row Publishers (2004)
3. Concepts and Models of Inorganic Chemistry – 3rd edition, B.E Douglas, D.H. Mc Daniel and Alexander, Wiley (2001)
4. Inorganic Chemistry – 2nd edition, D.F Shriver, P.W.Atkins and C.H.Langtore Oxford University Press (1994).
5. Chemistry of Elements – N.N. Greenwood and A.Earnshaw, Pergaman (2000).
6. Inorganic Chemistry – 2nd edition, C.E Housecraft and A.G Sharpe, Pearson Education Ltd. (2005).
7. Concise Inorganic Chemistry – J.D. Lee, ELBS

CHO HCT: 1.2: Stereo Chemistry and Reaction Mechanism – I

56 Hrs

UNIT-I

Bonding in Organic molecules and Aromaticity

Atomic and molecular orbits, concepts of bonding, anti bonding and non bonding molecular orbitals, hybridization – sp,sp^2 & sp^3, geometry and shape of simple molecules, bond length, bond angel and bond energies. Bonding in fullerenes, H-bonding. Bond polarity, dipole moment. Bonds weaker than covalent bonds, addition compounds, crown ethers, cryptonds, inclusion compounds, cyclodextrins, catananes, and rotaxanes.

Aromaticity in benzenoid and non benzenoid compounds, alternant, nonalternant hydrocarbons, Huckl's rule, annulenes. Aromaticity, antiaromaticity, nonaromaticity of organic systems(3-7 numbered rings & ring ions).

[14 hrs]

UNIT-II

Stereo Chemistry

Elements of symmetry, concepts of chirality, optical isomerism, projection formulae, Fisher, Saw horse, Newman and Flying wedge formulae and their inter conversion, optical isomerism due to one or more than one chiral centres.

Threo and erythro isomer, enantiomers, diastearic isomers and epimers. D-L and R-S conversions. Optical activity in the absence of chiral carbon – Biphenyls, allenes and spiranes, optical isomerism of nitrogen compounds , conformational analysis of (cyclic and acyclic systems) – ethane, propane, butane, mono & disubstited cyclohexanes.

Geometrical isomerism – cis-trans, syn-anti and E-Z nomenclature, isomerism in ketoximes and aldoximes, Beckmann rearrangement. [**14 hrs]**

UNIT-III

Reaction Mechanisms, Reactive Intermediates & Named reactions:

Types of mechanism, methods of determination of reaction mechanism – cross over experiments, product analysis, presences of intermediates, isotopic labeling, steriochemical evidences, thermodynamic and kinetic requirements, use of catalysts. Formation, structure and stability of carbocations, carboanions, free radicals, carbenes, nitrenes and aryne intermediates.

Name reactions and rearrangements – Aldol, Perkin, Dickman condensation, Hofmann, Schmidt, Lossen, Curtiurs rearrangements, Reimer-Tiemann reaction, Wittig reactions (Mechanism with examples). **[14 hrs]**

UNIT-IV

Pericyclic Reactions:

Definition, classifications of pericyclic reactions. Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene, 1.3.5-hexa triene and allyl systems. Woodward and Hoffmann correlation diagram. FMO & PMO approach, electrogatic reactions-conrotator and disrotatory motions, 4n, 4n+2 and allyl systems.

Cycloaddition – antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes. 1, 3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements, superfacial and antrafacial shifts of H., shifts involving carbon moieties, 3, 3-and 5, 5 – sigmatropic rearrangements, claisen, cope and azo cope rearrangements. **[14 hrs]**

REFERENCES

1. Advanced organic chemistry – Reaction mechanism & structure – Jerry March.
2. Reaction mechanism in organic chemistry – S.M Mukharji & S.P Singh
3. Advanced organic chemistry – C.K Ingld
4. A guide book to mechanism in organic Chemistry – Petersexes
5. Stereo chemistry of carbon compounds – E.L Eliel
6. Stereo Chemistry of carbon compounds – D. Nasipuri
7. Stereo Chemistry of carbon compounds – P.S Kalsi
8. Text book of organic Chemistry – I.L Finar, Vol- I & Vol-2.
9. Text book of organic Chemistry – R.T Marrison & R.N Boid.
10. Chemistry of natural products – Gurudeep Chatwal, Vol- I & Vol-2
11. Reactive intermediates in organic chemistry – N.S Isaacs
12. Named reaction in organic chemistry – Surrey
13. Named reaction in organic chemistry – Gurudeep Chatwal
14. Text book of advanced organic chemistry – B.S Bhal & Arun Bhal

CHP HCT: 1.3 Chemical Thermodynamics and Chemical Kinetics.

56 Hrs

UNIT-I

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, thermodynamic equations of state, limitations of Van't Hoff' s equation, Nernst Heal theorem & its applications. Third law of thermodynamics, determination of third law of entropies.

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 Ideal Solutions:

Deductions of laws of Raoult's ebullioscopy, cryoscopy and osmotic pressure. Quantitative treatment of Le-Chatelier principle.

Thermodynamics of Non-ideal Solutions: Activity, activity coefficient-standard states.

[14 hrs]

UNIT-II

Theories of Reaction Rates:

Activated complex theory and its applications to reactions in solution. Theory of unimolecular reactions- Lindeman, Hinsel-Wood and RRKM theory

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, linear free energy relationships - Hammett and Taft equations,. **[14 hrs]**

UNIT-III

Catalysis:

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

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. Mechanism of surface reactions. **[14 hrs]**

UNIT-IV

Electrochemistry - I

Electrochemistry of Solutions:

Ionic atmosphere, physical significance of k (Cuppa), Debye-Huckel theory to the problem of activity coefficient, Debye-Huckel limiting law, Debye-Huckel equation for appreciable concentration. The Huckel and Bronsted equation. Qualitative verification of Debye-Huckel equation, Debye-Huckel Onsager conductance equation, Bjerrum theory of ion association-triples ion-conductance minima.

[14 hrs]

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.

CSA CST: 1.4 Analytical Chemistry – I

56 Hrs

UNIT – I

Errors and Sampling:

Limitations of analytical methods, classifications of errors, accuracy, precision, minimization of errors, significant figures and computations, mean and standard deviation, distribution of random errors, relativity of results, confidence interval, comparison of results, comparison of the means of two samples, Paired t- test, the number of replicate determinations, correlation and regression, linear regression, comparison of more than two means (analysis of variance), Least square method, 6 sigma concept. Quality control and quality assurance. The basis of sampling, sampling procedure, sampling statistics, sampling and physical state, crushing and grinding, hazards in sampling. **[14 hrs]**

UNIT – II

Titrimetic and Gravimetric analysis:

Acid base titrations:

Principle, titration curves for strong acid - strong base, weak acid – strong base, weak base – strong acid, determination of equivalence point – theory acid base indicators, colour change range of indicator, applications for nitrogen, nitrates and carbonates estimation.

Complexometric Titrations:

Introduction, a simple complexation titration, titration curves, types of EDTA titrations, titrations of mixtures, selectivity, masking and demasking agents, metal ion indicators, some practical considerations.

Precipitation Titrations:

Precipitation reactions, titration curves, factors influencing the sharpness of end points, chemical indicators for precipitation titrations, applications of precipitation titration analysis.

Oxidation –Reduction Titrations:

Redox process, titration curves, redox indicators and applications.

Gravimetric analysis:

Requirements & conditions of precipitations, co-precipitation, post precipitation, nature of the precipitate, super saturation, precipitation from homogeneous solution and effect of excess of precipitant, temperature, pH and complex formation on completeness of precipitation. Filtration, washing of precipitates, drying and ignition of precipitates.

Organic Reagents in Inorganic Analysis:

Organic precipitants, general properties, reagents as precipitants. **[14 hrs]**

UNIT-III

Separation Techniques

Basic separation techniques in analysis, classification

Solvent Extraction:

Principle, distribution law, choice of solvents for extraction, synergic extraction, techniques-batch, continuous and multiple extractions and applications.

Paper and thin layer Chromatography:

General principles and classification of chromatographic methods-paper, thin layer, column and liquid chromatography.

Ion Exchange Chromatography:

Definitions, requirements for ion exchange resin, synthesis and types of ion exchange resins, principle, basic features of ion exchange reactions, ion exchange capacity, applications of ion exchange chromatography in preparative, purification and recovery processes, process of elution.

[14 hrs]

UNIT – IV

Conductometry :

Theory- Measurement of Conductivity - Basis for Conductometric titrations - Conductometry as an analytical tool.

Potentiometry :

Principles - Reference electrodes - indicator electrodes, selective electrodes - measurement of cell emf - potentiometric titrations.

Voltametry :

Polarography - Direct current Polarography - Theory - Dropping Mercury Electrode-Quantitative technique - Measurement of Wave Heights - Pulse Polarography - Rapid Scan Polarography - Stripping Voltametry - Cyclic Voltametry.

Amperometry :

Pricnciples, amperometric titrations with examples.

Elecrogravimetry:

Theory, completeness and nature of the deposit, instrumentation, electrolytic separation of metals and applications. **[14 hrs]**

REFERENCES

1. Fundamentals of Analytical Chemistry D.A Skoog, D.M West, Holler and Crouch, 8th edition, 2005, Saunders College Publishing New York.
2. Analytical Chemistry, G.D Christian, 5th edition, 2001, John Wiley and Sons Inc, India.
3. Vogel's Test book of Quantitative Chemical Analysis, J. Mendham, R.C Denny, J.D Barnes and M.J.K Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Educations Pvt. Ltd., New Delhi.
4. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
5. Instrumental Methods of Analysis, H.H Willas, L.L Merritt and J.A Deay, 7th edition, 1988.
6. Instrumental Methods of Analysis, W.M Dean and Settle, 7th edition, 1986, CBS Publishers, New Delhi.

Mathematics for Chemists:
CSM CST: 1.5 Mathematics and Computers for Chemists

[56 hrs]

UNIT – I

Matrix Algebra:

Matrix algebra, basic idea of inverse, adjoint, transpose and special matrices, matrix equation, Eigen functions and determents. Differential calculus- rules for differentiation, maxima and minima with respect to population of rotational energy levels, Bohar's radius, most probable velocity and Maxwell's exact and mexact differentials in thermodynamics properties. **[14 hrs]**

UNIT – II

Integration and Differentiation:

Basic rules of integration, partial differentiation, coordinate transformation (e.g Cartesian to spherical polar), elementary differential equations: variables – separable and exact first order differential equations, homogeneous, exact and linear equations, applications to chemical kinetics, secular equilibrium, quantum chemistry.

Fourier series, solutions of harmonic oscillator and Legendre equation, spherical harmonics, second order differential equation. Permutations and probability average root mean square and most probable errors with respect to kinetic theory of gases, least square curves fitting. **[14 hrs]**

UNIT – III

Computers for Chemists:

Introduction to computer and computing – basic structure, operating system, introduction to windows, data processing and principles of programming Flow charts. Introduction to computer languages (FORTAN & C), elements of computer languages, constants, variables, statements, operations and symbols. **[14 hrs]**

UNIT – IV

Computational Chemistry:

Programming in chemistry – developments of programmers involving simple formulae in chemistry, Vander Wall's equation, pH titration, dynamics, radioactive decay. Elementary structural features-bond angels, bond lengths, dihedral angles of molecules. Running standard programs and packages: linear regression, X-Y plot, differential equations, operation of packages – M.S Word, M.S Excel, Windows, ORIGIN and SIGMA programs. Recent trends in computer applications.
[14 hrs]

REFERENCES

1. The chemistry of mathematics – E.Staner, Oxford University Press.
2. Mathematics for chemists, Droggeti & Sucliffe, Longman.
3. Mathematical preparations for physical chemistry, F. Damiels, Mc Graw-Hill.
4. Chemical mathematics – D.M.Hist, Longman
5. Basic mathematics for chemists –Tebbutt, Willey .
6. Basic programming –Self Taught; Harch.
7. Computer programming :Shaum's outline series.
8. FORTRA-VI , V.Rajaraman.
9. Microcomputer quantum mechanics, J.P.Kilngbeck and Adan Hilger.
   An introduction to digital computer design-V.Rajaraman and T.Radhakrishanan,Prentice Hall.

PRACTICALS

CHI-HCP: 1.6 Inorganic Chemistry Practicals (any eight experiments)

1. Determination of iron using $KMnO_4$ (0.02M) and cerric ammonium sulphate (0.02M) as titrants.
2. Determination of calcium using $KMnO_4$ (0.02M) as titrants.
3. Determination of copper volumetrically using KIO_3 .
4. Estimation of calcium and magnesium carbonates in dolomite solution using EDTA titration.
5. Estimation of lead and tin in a mixture using EDTA titration.
6. Complexometric determination of a calcium and lead in a mixture.
7. Gravimetric analysis of sulphate with barium.
8. Gravimetric analysis of iron.
9. Determination of nickel gravimetrically using dimethyl glyoxime.
10. Separation and determination of two metal ions, iron and nickel, involving volumetric and gravimetric methods.
11. Separation and determination of two metal ions, copper and iron, involving volumetric and gravimetric methods.
12. Separation and determination of two metal ions, calcium and iron, involving volumetric and gravimetric methods. **[64 hrs]**

REFERENCES

1. A text book of quantitative inorganic analysis- A.I.Vogel, 3rd edition.
2. Vogel's text book of quantitative chemical analysis – J.Basset, R.C.Denney, G. H. Jeffere and J. Mendhom, 5th edition.
3. Quantitative chemical analysis – Daniel, C.Harris, 7th edition 2006.

CHO HCP: 1.7 Organic Chemistry Practicals

Preparations-two stage (Any 6 preparations from the following list)

1. Preparation of p-bromo aniline from analine.
2. Preparation of p-nitro aniline from analine.
3. Preparation of acetanilide from Acetophenone.(Beckmann Rearrangement)
4. Preparation of Benzanilide from Benzofinon
5. Preparation of 7-hydroxy-4methyl coumarin(Pechmann reaction).
6. Remier tiemann reaction (preparation of Salicyldehyde/B-hydroxynaphthadehyde)
7. Preparation of 2-4 dinitro benzene from benzene
8. Preparation of benzoic acid from toluene.
9. Cannizaros reaction.
10. Preparation of pthalimide from pthalic acid
11. Preparation of indigo from Anthranilic acid.
12. Preparation of s-benzyleiso thiouronium chloride.
13. Preparation of acetamide from acetophenone via oxime.

REFERENCES

1. Comprehensive practical organic chemistry preparation and quantitative analysis-Ahluwalia.V.K and Renu Agarval, University Press, Hyderabad (LCS edition 2000).
2. Comprehensive practical organic chemistry-quantitative analysis-V.K.Ahluwalia and university press-Hyderabad.
3. Advanced practical organic chemistry – N.K.Vishnu, second revised edition, Vikas Publication (2000).
4. Advanced practical organic chemistry – D.P.Agarwal, Goel Publishing house, Meerut (U.P).
5. Quantative & qualitative organic analysis, A.I.Vogel (CBS Publishers, New Delhi-2002).

HP HCP: 1.8 Physical Chemistry Practicals (any six)

1.Study of kinetics of hydrolysis of an ester using HCl/H_2SO_4 at two different temperatures, determination of rate of constants and energy of activation.

2.Study of kinetic reactions between $K_2S_2O_8$ and KI, first order, determination of rate constants at two different temperatures and Energy of activation.

3.Conductometric titration of mixture of HCl and CH_3COOH against NaOH.
4.Conductometric titration of mixture of HCl and CH_3COOH and $CuSO_4$ against NaOH.
5.Conductometry-To determine the degree of hydrolysis and hydrolysisconstant of aniline hydrochloride.
6. Conductometric titration of potassium iodide with mercuric perchlorate.
7. Phase diagram for Three component liquid system, acetic acid, benzene and water.
8. Kinetics of dissociation of trichloroacetic acid.

[64 hrs]

REFERENCES

1. Practical Physical Chemistry- A.J.Findlay.
2. Experimental Physical Chemistry-F.Daniel et el.
3. Selected Experiments in Physical Chemistry- Latham.
4. Experimental Physical Chemistry- Janes and Parichard.
5. Experimental Physical Chemistry- Shoemaker.
6. Experimental Physical Chemistry- Yadav, Goel Publishing House.
7. Experimental Physical Chemistry- Das R.C and Behera B., Tata Mc Graw Hill.

M.Sc. DEGREE IN CHEMISTRY

SECOND SEMESTER

CHI HCT: 2.1 Coordination Chemistry

56 Hrs

UNIT – I

Metal-Ligand Bonding:

Valance Bond Theory (VBT)-the electron-pair bond, the concept of effective atomic number, electronic configuration of metal complexes by VBT, draw backs of VBT.

Crystal Field Theory(CFT)-salient features, crystal field splitting of d orbitals in octahedral, tetrahedral, tetragonal and squarer planer field s Magnitude of Δ,factors affecting Δ, crystal field stabilization energy (CFSE), effects of crystal field splitting, energy of ligation, stabilities of oxidation states(Co^{III}). Spectrochemical series, nephelauxetic series, short comings of CFT, evidences for covalence, John-Teller distortion in metal complexes and metal chelates. M.O treatment of co ordination compounds involving σ and Π bonding. **[14 hrs]**

UNIT-II

Geometry, Magnetic and Spectral Properties of Metal Complexes:

Geometry of Metal Complexes:

Stereochemistry, coordination numbers, 3 to 8, isomerism in metal complexes, geometrical isomerism, optical isomerism, coordination isomerism, ionization isomerism, linkages isomerism.

Magnetic Properties of Metal Complexes:

Magnetic susceptibility, types of magnetic behavior, diamagnetic corrections, orbital contribution, spin-orbit coupling, ferro and anti-ferromagnetism.

Spectral Properties of Metal Complexes:

Term symbols, selection rules for electronic transitions-spin selection rule, the Laportic selection rule, Orgel diagrams, Tanabe-Sugano diagrams, stereo isomerism, chirality, CD, ORD, Cotton effect and magnetic circular dichroism, absolute configuration. [**14 hrs]**

UNIT-III

Metal-Ligand Equilibria in Solution:

Step-wise and over-all formation constant and their relationships, trends in step wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate and macro cyclic effects and their thermodynamic origin, determination of binary formation constants by pH meter, spectrophotometry, polarography and by ion exchange methods.

Kinetics and Mechanism of Reactions of Coordination Compounds:

Introduction, inert and labile complexes. Mechanism of substitution reactions, classification of ligand substitution reactions in octahedral and square planar complexes, molecular rearrangements of four and six coordinated complexes.

Electron Transfer Reactions (Redox Reactions):

Inner and outer sphere mechanisms, one electron, two electron, complimentary and non complimentary electron-transfer reactions. [**14 hrs]**

UNIT IV

Chemistry of Inorganic materials

Synthesis of bulk materials, Chemical deposition, defects and ion transport, metal oxides, nitrides and fluorides, chalcogenides, chevrel phases and thermoelectric, Framework structures, hydrides and hydrogen storage materials, Inorganic pigments, molecular materials and fullerides. [**14 hrs]**

REFERENCES

1. Basic Inorganic Chemistry, F.A.Cotton, G.wilkinson and P.L.Gau, Jhon Wiley and sons, Inc, 6th edition,1999.
2. Inorganic Chemistry,J.E.Huheey, E.A.Keiter and R.L.Keiter, 4thedn 1993.
3. Chemistry of the Elements, N.N.Greenwood and A.E.Earnshaw, Buttrerworth Heilemann,1997.
4. Esseutial Ternds in Inorganic Chemistry, D.M.P.Mingos, Oxford univ press 1998.
5. Magnetochemestry, R.L.Carlin, Springer Verlag.
6. Coordination Chemistry, Fred Basolo and Ronald C. Johnson, Wiley, New York, 1984.
7. Chemistry of Complex Equilibria, M.T Beck, Rinhold, London, 1990.
8. Concise Coordination Chemistry, R Gopalan and V Ramalingam, Vikas Publishing House Pvt Ltd., New Delhi, 2005.
9. Shriver and Atkin's Inorganic Chemistry, Atkins, Overton, Rourke, Weller, Armstrong, 5th Ed, Oxford University press, 2012

CHO HCT: 2.2 Heterocyclic Chemistry, Natural Products Reagents in Organic Synthesis

56 Hrs

UNIT-I

Heterocyclic Chemistry:

IUPAC nomenclature of heterocyclic ring systems (3-7 memberd rings and simple fused systems) comparative aromaticity of pyrrole, furon, thiophene, pyridine. Methods of synthesis, electorphilic and nucleophilic substitutions reactions of pyrrole, furon, thiophene, pyridine ring systems. Compression of basecity of pyridine, piperidine and pyrrole.

Fused heterocycles of 6 & 5 memberd rings-synthesis and reactions of indole, benzofurn, quinoline, isoquinoline with special references to Fischer indole synthesis, and Skraup synthesis, Bischler-Napier Laski synthesis, mechanism of electorphilic substitution reaction of indole, quinoline and benzofuran. **[14 hrs]**

UNIT-II

Chemistry of Natural Products Alkaloids Terpenoids and steroids.

Alkaloids – classifications occurrence, general methods of structural elucidation, stereo Chemistry and synthesis of quinine, papareine, morphine.

Terpenoids – occurrence general methods of structural elucidation, stereo Chemistry and synthesis of following representative molecules-citral, camphor and santonin.

Steroids – cholesterol, ergosterol-structure and synthesis. **[14 hrs]**

UNIT-III

Carbohydrates, Proteins and Nucleic acids

Carbohydrates-determination of ring structures of mono sacharides and di sacharides with reference to glucose, fructose, maltose and sucrose.

Proteins – Amino acids, peptides, peptide synthesis using blocking reagents, modern methods of peptide synthesis. Structure of proteins – primary. secondary & tertiary structure, sequence of amino acids in proteins, end group analysis.

Nucleic acids- chemical and enzymatic hydrolysis of nucleic acids, purine & pyrimidine bases, double helix of DNA, base pairing via H-bonding, various types of RNA & their functions.

[14 hrs]

UNIT-IV

Reagents in organic synthesis:

Use of following reagents in organic synthesis and functional group transformation

i) Dicyclohexylcarbodiimide (DCC)
ii) Tri-n-butyltin hydride
iii) Wood ward and Pre Vost hydroxylation
iv) Osmium tetroxide
v) DDQ
vi) Selinium dioxide
vii) Phase transfer catalysis
viii) Crown ethers
ix) Merrifield resin
x) Peterson's synthesis
xi) Lithium aluminum hydride
xii) Wilkinson's catalyst
xiii) Gilman's reagent
xiv) Zigler-Natta catalyst

[14 hrs]

REFERENCES

1. Pericyclic Reactions-S.M.Mukharji and Singh S.P
2. Heterocyclic Chemistry- J.Joule and Smith
3. Introduction to Chemistry of heterocyclic compounds
4. Heterocyclic Compounds – Raj Bansal

5. Textbook of Organic Chemistry-R.J.Moorism and Boyd
6. Text book of Advanced Organic Chemistry-Arun Bhal

CHP HCT: 2.3 Electro-, Quantum- and Photochemistry

56 Hrs

UNIT-I

Electrochemistry - II

Electrochemistry

Debye-Huckel theory of strong electrolytes, Debye Huckel – Onsager equation, Debye – Huckel limiting equation for activity coefficients, modifications and verifications. Electrical double layer and its thermodynamics. A brief survey of Helmholtz – Perrin, Gouy – Champman and Stern electrical double layer, EMF cells, liquid junction potential and its determination. Energetics of cell reactions, effect of temperature, pressure and concentration on energetics of cell reactions (Calculation of ΔG, ΔH and ΔS)Electrochemical energy sources – Batteries, classification, characteristics, primary, secondary and Fuel cells. **[14 hrs]**

UNIT-II

Irreversible Electrode Process:

Introduction, reversible and irreversible electrodes. Polarization, Ohmic overvoltage, concentration overvoltage, activation overvoltage. Hydrogen over voltage and oxygen over voltage. Effect of temperature, current density and pH on over voltage. Experimental determination of over voltage. Equations for concentration over potential, diffusion current, stationary current, potential curves, thickness of diffusion layer, diffusion controlled current potential curves at a dropping mercury electrode, polarography, half wave potential, application in qualitative and quantitative analysis. Energy barrier and electrode kinetics, Buttler-Volmer equation, Tafel equation. **[14 hrs]**

UNIT-III

Quantum Mechanics:

Wave – particle duality of material particles, de Broglie equation, Heisenberg uncertainty principle. Concept of operators (operator – operand), algebra of operators, commutative and non commutative operators, linear operators, Laplacian operator, Hamiltonian operator, Eigen value, Eigen function, Hermitian operator, turn over rule, atomic units. Wave equation for stretched rings Schrodinger wave equation for particles. Postulates of quantum mechanics. Application of Schrodinger equation to a free particles and to a particle trapped in a potential field (one dimension & three dimension). Degeneracy, wave equation for H-atom separation and solution of R, ϕ and Θ equations. Application of Schrodinger equation to rigid rotator and harmonic oscillator. Approximate methods-necessity of approximate methods, perturbation method, the theory of perturbation method-first order and second order correction, application to He – atom

(first order correction only)-calculation of first ionization potential and binding energy. Variation theorem statement and proof. **[14 hrs]**

UNIT-IV

Photochemistry:

Introduction to photochemistry, quantum yield and its determination, factors affecting quantum yield, actinometry-uranyloxalate and potassium ferrioxalate actinometres, acetone and diethylketone actinometres. Term symbols and significance. Photosensitization: by mercury, dissociation of H_2, photochemical kinetics of: decomposition of CH_3 CHO, formation of HCl. Photodegradation: photocatalyst-ZnO, TiO_2, principle, application of ZnO/TiO_2 in the photodegradation of dyes(IC), pesticides(DDT) and in industrial effluents. Effect of photodegradation on COD values. **[14 hrs]**

REFERENCES

1. Elements of physical chemistry – Lewis and Glasstone.
2. Physical chemistry –P.W.Atkine, ELBS, fourth edition 1990.
3. Basic physical chemistry –W.J.More.
4. Physical chemistry-G.M.Barrow.
5. Introduction to electro chemistry-S.Glastone.
6. Modern electro chemistry, vol I & II, J.O.M.Bockris and A.K.N.Reddy, 1970.
7. Electrochemistry-principles and applications-E.G Potter.
8. Quantum chemistry- A.K Charlra, second edition, 1983.
9. Quantum chemistry-Eyring, Walter and Kimball, John Wiley and Sons.
10. Quantum chemistry-R.K Prasad, 1996.
11. Advances in photochemistry by Rohatgi # Mukharjee
12. Principles and applications of photochemistry by R.P.Wayne Elesvier New York 1970
13. Molecular reactions and photochemistry by Dupey & Chapman, Prenctice Hall international, Tokyo, 1972

CSA-CST 2.4: Analytical Chemistry-II

[56 hrs]

UNIT-I

Flame Photometry and Atomic Absorption Spectrometry:

Principles and Theory - Instrumentation - Flames - Burners - Nonflame Techniques - Spectral and Chemical Interferences - Experimental Aspects.

Atomic Emission Spectrometry and Inductively Coupled Plasma:

Principles and Instrumentation - Excitation source - Limitations of AES - Principles of Plasma Spectroscopy - Excitation Source in ICP -Applications.

Nephelometry and Turbidometry:

Tyndall, Rayleigh and Raman Scattering - Principles, Instrumentation and Applications.

[14 hrs]

UNIT-II

Molecular Luminescence:

Principles of Fluorescence and Phosphorescence - Fluorimetry in Chemical Analysis - Instrumentation in Fluorimetry - Fluorescence and Chemical Structure and - Fluorescence in quenching and inner filter effect - Phosphorescence Spectroscopy – Jablonski diagram- Phosphorescence and Chemical Structure - Phosphorimetry in Quantitative Analysis.

Chemiluminescence:

Principles, measurement of Chemiluminescence - Quantitative Analysis - Titrations - Electrochemiluminescence.

Polarimetry and Related Methods :

Polarized light - Applications of Polarimetry - Optical Rotatory Dispersion and Circular Dichroism –cotton effect, Instrumentation in ORD and CD. **[14 hrs]**

UNIT-III

Thermal Methods of Analysis

Thermo Gravimetric Analysis:

Introduction, thermo gravimetric analysis(TGA) – types of thermo gravimetric analysis, principles, factors affecting the results – heating rate, furnace instrument control/data handling. Applications-purity and thermal stability, evaluation of correct drying temperature, analysis of complex mixture and determination of kinetic parameters of thermal degradation.

Differential Thermal Analysis (DTA):

Theory , variables affecting the DTA, general principles, instrumentation, applications – analysis of the physical mixtures and thermal behavior study, determination of decomposition point.

Differential Scanning Calorimetry (DSC):

Basic principle, differences between DTA and DSC, instrumentation – power compensated DSC, heat flux DSC, applications – studies of thermal transistors and isothermal crystallization, pharmaceutical industry for testing the purity of the samples. Thermometric titrimetry and direct injection enthalpimetry-principle, instrumentation, applications. **[14 hrs]**

UNIT-IV

Electroseparation techniques:

Supercritical fluid chromatography: Introduction, Properties of supercritical fluids, Instrumentation, and applications.

Electrophoresis: Principle, classification, capillary electrophoresis, , Instrumentation, Application to capillary zone electrophoresis, gel electrophoresis.

Electroosmosis: Principles, Instrumentation and applications.

Field flow fractionation: Separation mechanisms, Methodology, Advantages over chromatographic methods. **[14 hrs]**

REFERENCES

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th ed., 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 prentice Hall, Inc. New Delhi.

4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint.2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders CollegePublishing, California, 1990.
6. Principles and Practicals of Analytical Chemistry, F. W. Fifield and Kealey,3rd edition, 2000, Blackwell Sci., Ltd. Maiden, USA.
7. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
8. Introduction to Instrumental Analysis, Robert. D. Braun, Pharm. Med. Prem. India, 1987.
9. Instrumental Method of Analysis, W. M. Dean and Settle, 7th edition, 1986, CBS Publishers, New Delhi.
10. Instant Notes of Analytical Chemistry, Kealey and Haines, Viva books Pvt. Ltd., 2002.
11. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
12. Principles and Practice of Analytical Chemistry, F. W. Fifield and Kealey, 5th edition, 2000, Blackwell Sci., Ltd. Maiden, USA.
13. Basic Concepts of Analytical Chemistry, S.M.Khopkar, New Age Intrenational.
14. Elements of X-Ray Crystallography, L.V.Azaroff, McGraw Hill.
15. X-Ray Crystallography, M.J.Buerger, John Wiley.
16. Elements of X-Ray Diffraction,B.D.Cullity.
17. An Introduction to X-Ray Crystallography, M.M.Woolfson Cambridge University Press.
18. The Basics of Crystallography and Diffraction, Christopher Hammond, Oxford Science Publications.

CSB SCT: 2.5 SELECTED TOPICS IN CHEMISTRY- I

[56 hrs]

UNIT-I

Amino Acids: General structure, Physiological properties

Peptides: Structure and conformation of peptide bond, peptide synthesis: Solution phase and Merrifield's solid phase synthesis, Racemization and use of HOBt, Synthesis of oxytocin and vasopressin, biological importance of insulin, selective cleavage of polypeptide bonds (chemical and enzymatic).

Proteins: Structure determination: C and N terminal residue determination, primary, secondary, tertiary and quartenary structure determination, denaturing and renaturing of proteins.

Nucleic acids: Introduction, structure and synthesis of nucleosides and nucleotides, protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions.
Methods of formation of internucleotide bonds: DCC, phosphodiester approach and phosphoramide methods. Solid phase synthesis of oligonucleotides. Structure of RNA and DNA, Crick-Watson model, role of nucleic acids in the biosynthesis of proteins.
Genetic code, replication of DNA. [**14 hrs]**

UNIT - II

Carbohydrates: Introduction, Ring size determination of monosaccharides, configuration and conformations of monosaccharides, anomeric effect, Hudson's rules, epimerization and mutarotation.

Synthesis, industrial and biological importance of glycosides, amino sugars, sucrose, maltose and lactose.

Polysaccharides: General methods of structure elucidation. Industrial importance and biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar.

Photosynthesis and biosynthesis of carbohydrates.

Lipids: Nomenclature, classification, purification, synthesis of lipids, phospholipids, sphingolipids, biological importance of lipids: Lecithin, sphingolipids, oils and fats.

Prostaglandins: Introduction, classification and biological importance, constitution of PGE1.

[**14 hrs]**

UNIT - III

Chemometrics

Introduction to Chemometrics, principles of experimental design, factorial and fractional factorial design, Specific applications. Response surface methodology and Optimization, Response surface designs, Sequential optimization, specific, numerical problems. Modelling and Knowledge processing: multiple linear regressions, test parameter estimation, PCR PLS, PCA etc. Cluster analysis and descriminant analysis, modelling of multiway regression, A I and expert systems, Neural Networks, Fuzzy theory, Genetic Algorithms approach for Analytical Chemistry applications. [**14 hrs]**

UNIT-IV

Research Methodology

Introduction: Nature and importance of research - aims, objective, principles and problems - selection of research problem - survey of scientific literature - primary and secondary sources - citation index for scientific papers and journals - patents.

Conduct of Research work : Physical properties useful in analysis and methods of separation prior to analysis - Isolation techniques - extraction - Soxhlet extraction, crystallization, sublimation - methods for vacuum sublimation and distillation under reduced pressure. Chemistry of working with hazardous materials - acid / water sensitive, corrosive, toxic, explosive and radioactive materials. [**14 hrs]**

References:

1. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. K. Albert, L. Lehninger, D.L. Nelson, M.M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
3. Harper's Biochemistry, Ed. R.Harper, 22nd edition, Prentice Hall Press, New York, 1990.
4. Encyclopedia of Chemical Technology – Kirck-Othmer series
5. Harper's Review of Biochemistry – P.W. Martin, P.A. Mayer and V.W. Rodfwell, 15th

edition, Maurzen Asian Edition, California, 1981.
6. Brian R. Eggins, Chemical Sensors and Biosensors, Analytical Techniques in the Sciences (ANTS), 2nd Edition, Wiley, 2002.
7. Gabor Harsanyi, Sensors in Biomedical Applications - Fundamentals, Technology and Applications, CRC Press, 2000.
8. Raluca-Ioana Stefan, Electrochemical Sensors in Bioanalysis, CRC Press, 2001.
9. Susan R. Mikkelsen and Eduardo Cortón, Bio Analytical Chemistry, John Wiley & Sons Inc, 2004
10. Andreas Manz and Nicole Pamme, Bio Analytical Chemistry, Imperial College Press, 2012
11. J. Anderson, H.M. Durston and M.Poole, Thesis and assignment writing - Wiley Eastern Ltd., (1970).

OPEN ELECTIVE/ CROSS BORDER
PAPER-I
(NON CHEMISTRY STUDENTS ONLY)
PAPER –I
OET SCT: 2.1 ENVIRONMENTAL CHEMISTRY

28 Hrs

UNIT-I

Air Pollution:

Types and sources of air pollutants; natural background, concentrations of air pollutants; principles and methods of sampling; a survey of reactions and methods involved in the determination of carbon dioxide, sulphur dioxide, nitrogen oxides, hydrocarbons & particulates; consequences of air pollution.

Radioactive Pollution:

Sources of pollutants; effect of vegetation and health. Detection and monitoring of radioactive pollutants. Methods of safe disposal of radioactive waste. **[14hrs]**

UNIT-II

Water Pollution:

Origin of waste water, types of water pollutants and their effects; sources of water pollution; domestic, industrial and agricultural soil has source of pollution. Objectives of analysis. Parameters of analysis; color, turbidity, total solids, conductivity, acidity, alkalinity and hardness, chloride, sulphate, fluoride, silica, phosphate and different forms of nitrogen.

Heavy Metal Pollution:

Public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey in instrumental techniques for the analysis of heavy metals in aquatic systems; pesticides as water pollutants and their analysis; water pollution laws and standards.

[14 hrs]

REFERENCES

1. Standard Methods for Chemical Analysis, A.J Welcher (Part-B), Robort E Kiegor Publishing Co., USA, 1975.
2. Environmental Chemistry, S.E Manahar, Willard Graut Press, London, 1983.
3. Environmental Chemistry, A.K De, Wiley Eastern Publishers.
4. Environmental Chemistry, B.K Sharma, Himalaya Publishing House.
5. Environmental Chemistry, C. Baird & W.H Freeman.

OET SCT: 2.2 INORGANIC AND PHYSICAL CHEMISTRY

UNIT-I

Periodic Properties:

Atomic size, ionic radii, ionization potential, electron affinity and electro negativity. Applications of electro negativity.

General Characteristics of s, p, d and f -block Elements:

Comparative study with reference to electronic configuration, oxidation states, chemical properties, spectra and magnetic properties of d- and f- block elements. Survey of essential and trace elements in biological systems.

Chemical Bonding:

Ionic bond- size effect and solubility. Covalent bond- simple binary systems, hydrogen bond- water and in biological systems.

Concepts of Acids and Bases:

Arrhenius, Bronsted-Lowry, Lewis, Lux-Flood and solvent system concepts.

Non-aqueous Solvents:

Classification of solvents, properties of solvents (dielectric constant, donor and acceptor properties),protic (anhydrous **H_2SO_4 and** acetic acid) and aprotic solvents (liquid $S0_2$ and **N_2O_4).**

[14 hrs]

UNIT-II

Microwave Spectroscopy:

Rotation spectra of diatomic molecules. Applications - Principles of determination of bond length and moment of inertia from rotational spectra.

Infrared Spectroscopy:

Vibration of diatomic molecules, vibrational energy curves for simple harmonic oscillator. Theory of infrared absorption. Types of absorption, intensity of absorption bands. Number of fundamental vibrations and theoretical group frequencies. Identification, interpretation of infrared spectra - correlation chart. Important spectral regions, characterization of functional groups and structure determinations - CO_2 and H_2O, CH_3COCH_3 .

Applications of Physical Chemistry:

Concepts of entropy and free energy. Partial molar volume and its determination by density measurements. Symmetry elements and symmetry operations with examples of simple molecules. X-ray diffraction. Bragg equation and Miller indices. Order of a reaction and its determination. Energy of activation and its determination. Assumptions of activated complex theory. Fast reactions with examples. Polymers and their classification. Arrhenius theory of strong and weak electrolytes. Assumptions of Debye-Huckel theory of strong electrolytes. Types

of electrodes. Corrosion and its prevention. Laws of photochemistry. Quantum yield and its determination, photodegradation. **[14hrs]**

REFERENCES:

1. Inorganic Chemistry, 3rd edn., G.L. Miessler and D.A. Tarr. Pearson Education (2004).
2. Inorganic Chemistry, 2nd edn., D.F. Shriver. P.W. Atkins and C.H. Langford, Oxford University Press (1994).
3. Inorganic Chemistry, 2nd edn., C.E. Housecraft and A.G. Sharpe, Pearson Education Ltd. (2005).
4. Basic Inorganic Chemistry - 3rd edn., F.A. Cotton, G. Wilkinson and P.L . Gaus, John Wiley and Sons (2002).
5. Inorganic Chemistry, 3rd edn., James E. Huheey, Harper and Row Publishers (1983).
6. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash. 4th edition, Tata McGraw-Hill, New Delhi.
7. Introduction to Spectroscopy- Pavia, Lampman and Kriz, 3rd edition, Thomson.
8. Spectroscopy, B. P. Straughan and S. Walker. John Wiley & Sons Inc., New York, Vol. 1 & 2, 1976.
9. Vibration Spectroscopy Theory and Applications, D. N. Satyanarayana, New Age International, New Delhi.
10. Organic Spectroscopy, William Kemp, 3rd edition. Palgrava. 1991. 1 I. Chemical Kinetics by K.J. Laidler.
11. Chemical Kinetics – K.J.Laidler.
12. Chemical Kinetics-Moore and Pearson.
13. Kinetics and Mechanism of Chemical Transformation - J. Rajaram and J.C. Kuriacose.
14. Introduction to Electrochemistry by S. Glasstone.
15. Thermodynamics for Chemists by S. Glasstone. Affiliated to Liasl-West Press. New Delhi, (1965).
16. Advances in Photochemistry - Rohatgi Mukherjee.
17. Principle and Applications of Photochemistry - R.P Wayne. Elsevier, New York. (1970).
18. Elements of Physical Chemistry - Glasstone and Lewis.

CHI HCP: 2.6 Inorganic Chemistry Practicals (Any six)

1. Analysis of sodium carbonate and sodium bicarbonate in baking soda by acid-base titration.
2. Determination of calcium in lime stone solution by redox titration.
3. Determination of total hardness, calcium and magnesium hardness and carbonate and bicarbonate hardness of water by complexometric titration using EDTA.
4. Determination of percentage of chloride by precipitation titration-Mohr, and Volhard methods.
5. Analysis of copper in alloy solution by iodometric titrations.
6. Flame emission spectrophotometric determination of sodium and potassium in pond/lake waters.

REFERENCES

1. A text book of quantitative inorganic analysis- A.I.Vogel, 3rd edition.
2. Vogel's text book of quantitative chemical analysis – J.Basset, R.C.Denney, G. H. Jeffere and J. Mendhom, 5th edition.
3. Quantitative chemical analysis – Daniel, C.Harris, 7th edition 2006.

CHO HCP: 2.7 Organic Chemistry Practicals (Any six)

Systematic qualitative analysis of organic binary mixture (solid + solid) with derivative preparation (min six mixtures)

NOTE: In the examination, candidate has to separate the binary mixture and analyse one component indicated by the examiner.

REFERENCES

1. Comprehensive practical organic chemistry preparation and quantitative analysis-Ahluwalia.V.K and Renu Agarval, University Press, Hyderabad (LCS edition 2000).
2.Comprehensive practical organic chemistry-quantitative analysis-V.K.Ahluwalia and university press-Hyderabad.
3.Advanced practical organic chemistry – N.K.Vishnu, second revised edition, Vikas Publication (2000).
4. Advanced practical organic chemistry – D.P.Agarwal, Goel Publishing house, Meerut (U.P).
5. Quantative & qualitative organic analysis, A.I.Vogel (CBS Publishers, New Delhi-2002).
6. Fundamentals of Analytical Chemistry-D.A.Skoog, D.M.West, Holler and Crouch, 8th edn., Sunders College Publishing, New York, 2005.
7. Quantitative Analysis-R.A.Day and A.L.Underwood, 6th edn., 3rd Indian Regrint, Pearson Education Pvt. Ltd., New Delhi, 2003.
8. Vogel's Textbook of Quantitative Chemical Analysis, J.Mendhan, R.C.Denny, J.D Barnes and M.J.K Thomas, 6th edn., 3rd Indian Regrint, Pearson Education Pvt. Ltd., New Delhi, 2003.
9. Analytical Chemistry, G.D Christian, 5th edn., John Wiely & Son's, Inc., India, 2001.
10. Analytical Chemistry Principles, John H.Kennady, 2nd edn., Saunders College Publishing, California, 1990.

CHP HCP: 2.8 Physical Chemistry Practicals (any six)

1. Potentiometric titration of KI vs $KMnO_4$ solution.
2. Potentiometric titration of Fe(II) vs Ce(IV).
3. To obtain the absorption spectra of colored complexes, verification of Beer's law and estimation of metal ions in solution using spectrophotometer.
4. Spectrophotometric titration of $FeSO_4$ against $KMnO_4$.
5. Adsorption of acetic acid on charcoal
6. Adsorption of Oxalic acid on activated charcoal
7. Conductometric determination of degree of hydrolysis and hydrolysis constant of aniline hydrochloride

8. Determination of dissociation constant of weak acid by potentiometric method
9. Potentiometric determination of equivalent weight and K_a for a weak acid.

[64 hrs]

REFERENCES

1. Practical Physical Chemistry- A.J.Findlay.
2. Experimental Physical Chemistry-F.Daniel et el.
3. Selected Experiments in Physical Chemistry- Latham.
4. Experimental Physical Chemistry- Janes and Parichard.
5. Experimental Physical Chemistry- Shoemaker.
6. Experimental Physical Chemistry- Yadav, Goel Publishing House.
7. Experimental Physical Chemistry- Das R.C and Behera B., Tata Mc Graw Hill.

M.Sc., DEGREE IN CHEMISTRY
THIRD SEMESTER

CHS HCT: 3.1 Spectroscopy – I
(Group Theory, Symmetry & Molecular spectroscopy)

[56 hrs]

UNIT – I

Group Theory and Symmetry:

Symmetry elements & Symmetry operations, groups, subgroups, cyclic groups conjugate relationships, classes, molecular point groups, Schoenflies notations, matrix representations of symmetry operation, matrix representations of groups, Reducible and Irreducible representations, characters of representations, The great orthogonality theorem, character tables and their construction (C_{2v}, C_{2h}, C_{3v})– Mullikan symbols, molecular models. Determination of vibration modes, hybridization, molecular orbitals on the basis of group theory. **[14 hours]**

UNIT – II

Electromagnetic radiation

Characterization – quantization of energy levels – regions of electromagnetic radiation spectrum – interaction electromagnetic radiation with matter – representation of spectra-intensity and width of spectral lines.

UV-Visible Spectroscopy: Quantitative aspects of absorption – Beer- Lambert's law. Terminology associated with absorption measurements. Criteria for spectrophotometric determinations with examples (Fe, Mo and Ni). Limitations of the law, Types of absorption bands, modes of electronic transitions, simple chromophoric –auxochrome theory, solvent effect and choice of solvent. Prediction of λ-max value by using Wood-Ward and Fieser rules for conjugated diens, trienes and cyclic α, β unsaturated aldehydes and ketones, Instrumentation (single beam and double beam spectrophotometers). Quantitative applications of UV-Visible spectroscopy in structural determination. **[14 Hours]**

UNIT – III

Microwave Spectroscopy

The rotation of molecules – rotation spectra of diatomic molecules – the rigid diatomic molecule – rotational energy levels – selection rules – effect of isotopic substitution – the non rigid rotator – spectrum of a non rigid rotator – polyatomic linear molecules – techniques and instrumentation.

Vibrational Spectroscopy

Vibrating diatomic molecule – simple harmonic oscillator – vibrational energy levels – anharmonic oscillator selection rules – fundamental vibrations, overtones and hot bands – diatomic vibrator rotator, vibration rotation spectra of carbon monoxide – interaction of rotation and vibration – Born – Oppenheiner approximation – FT – IR Spectrometer.

Raman Spectroscopy:

Classical theory of Raman Effect – rotational Raman spectra – Linear – Vibrational Raman Spectra – Instrumentation. **[14 Hours]**

Unit IV

X-Ray Diffraction:

Production of X-Rays - Measurement of X-Rays Principles of X-Ray absorption - Principles and instrumentation in X-Ray fluorescence.

X-Ray diffraction - Bragg's laws - Miller indices laws - transmission and reflection method - Debye Scherrer method - single crystal and polycrystalline diffraction studies. Electron microprobe – principles and instruments – principles of electron diffraction - working of SEM and TEM.

Photoelectron Spectroscopy:

Basic principles-photoelectric effect, ionization-process, Koopman's theorem-photoelectric spectrum of simple molecules, ESCA-chemical information from ESCA. **[14 Hours]**

REFERENCES:

1. Physical Methods in Inorganic chemistry, R.S. Drago, East-West Press
2. Structural Methods in Inorganic chemistry, EAV Ebsworth, David W H Eankin Stephen Cradock, Blackwell scientific publications.
3. An introduction to Magnetic Resonance spectroscopy, D.N. Sathyanarayana, I.K. International.
4. Rotational and Vibrational Spectroscopy D.N. Sathyanarayana, I.K. International.
5. Chemical Applications of Group Theory, F.A. Cotton, John – Wiley.
6. Symmetry and Molecular Spectroscopy, K. Veerareddy, New age international.
7. Molecular Spectroscopy, G. Aruldhas, Prentice Hall, India.
8. Fundamentals of Molecular Spectroscopy, C.N. Barnwell, Tata McGraw Hill.
9. Fundamentals of Molecular Spectroscopy, G.M. Barrow McGraw Hill.

CHS HCT: 3.2
NUCLEAR CHEMISTRY AND MATERIALS SCIENCE

56 Hrs

NUCLEAR CHEMISTRY

UNIT – I

The Atomic nucleus – Elementary Particles – The Quarks – Classification of Nuclides – Nuclear Stability – Mass Defect and Binding Energy.

Nuclear models: Shell model – Liquid drop model – Fermi Gas Model – Optical Model.

Radioactivity: Radioactive elements, general characteristics of radioactive decay, interaction of α, β and γ – rays with matter.

Units of Radioactivity and its measurements: Units – scintillation counter – ionization Counter – Proportional Counter – G.M. counter – Neutron Detectors. **[14 Hours]**

UNIT – II

Induced Radioactivity – Nuclear Reactions – Types of nuclear reactions – Reaction Cross-section – Compound Nucleus Theory – specific nuclear reactions – Transuranium Elements – Photonuclear Reactions.

Nuclear Fission – Process of Fission – Fission fragments and their mass distributions – Charge Distribution – Fission energy – Theory of nuclear fission – Neutron evaporation & Spallation – Nuclear Fusion – Thermonuclear Reactions.

Nuclear Reactors: Classification – Critical size of a reactor – Power Reactor – Breeder reactor - Reprocessing of spend fuels – Nuclear waste management.

Applications of Nuclear Chemistry: Chemical investigation – Analytical applications – Age determinations – Radio dating – Neutron Activation Analysis – Application in medical field.

[14 Hours]

Materials science

UNIT – III

Atomic packing in crystals – Rules governing atomic packing – effect of radius ratio – Pauling's rules & its application to actual structure – Polymorphism, Isomorphism & solid solutions.
Imperfections in atomic packing – Types – Point defects, line defects & plane defects.
Mechanical Properties of Crystals – Classification of properties – Properties of engineering importance – Anisotropy in crystals – Elastic deformation – Plastic deformation.
Phase Diagrams and Phase Transitions: One Component – Two components – Three component Systems – Simple and Binary Systems – Classification of Phase Transitions – Representation of Phase Transitions – Factors Influencing Rate of Phase Transitions.

[**14 Hours]**

UNIT – IV

Electronic Properties and Band Theory

Introduction: Metals, Insulators and Semi conductors – Electronic Structure of Solids – Band Theory – k space and Brilliouin zones – Band structure of metals, insulators and semi conductors – Applications of semi conductors.

Magnetic Properties: Behaviour of substances in a magnetic field – Effect of Temperature – Mechanism of ferro – and antiferro magnetic ordering – Permanent Magnets.
Optical properties – Luminescence and Phosphorescence – Lasers – Ruby Laser and neodium lasers.

Organic Solid State Chemistry

Electrically conducting organic solids – Organic metals – Conjugated systems – Doped poly acetylene – Polyparaphenylene – Polypyrrole – Organic Charge Transfer complexes and new Super conductors. **[14 Hours]**

RFERENCES:

1. Nuclear Physics by I. Kaplan, Addison – Weley, Reading Mass, 1963 (IBH).
2. Nuclear Chemistry, Choppin and Rydberg, Pergamon Press.
3. Nuclear and Radiochemistry, G. Friedlander, J.W. Kennedy, E.S. Macias and J.M. Miller, Wiley Interscience, NY.
4. Essentials of Nuclear Chemistry, H.J. Arnikar New Age International.
5. Introduction to Solids, Leonid V. Azaroff, Tata McGraw-Hill New Delhi
6. Solid State Chemistry and its Applications, Anthony R West – John Whiley and Sons
7. Inorganic Chemistry, C.S.G. Philips and R.J.P. Williams, Oxford Press
8. The Structure and Properties of Materials, R.M. Rose, L.A. Shepard and J.Wulff, Wiley.
9. Introduction to Magnetochemistry, A. Earnshaw, Academic Press.
10. Advanced Inorganic Chemistry, F.A. Cotton and G. Wilkinson, Wiley

11. Callister's Material Science and Engineering, R.Balasubramanyam, Wiley and Sons.
12. New Directions in Solid State Chemistry, CNR Rao and J. Gopalkrishnan, Cambridge University Press.

CHP HCT: 3.3 :Advanced Physical Chemistry

56 Hrs

UNIT – I

Statistical Thermodynamics:

Concepts of distribution, thermodynamic probability and most probable distribution, Maxwell-Boltzmann distribution law. Partition functions – translational, rotational, vibrational electronic partition functions. Calculation of thermodynamic properties in terms of partition functions. Applications of partition functions. Chemical equilibrium and equilibrium constant in terms of partition functions. Fermi – Dirac Statistics – distribution law and applications to metal. Bose-Einstein statistics – distribution law and application to solids.

Ensemble averaging postulates of ensemble averaging. Canonical, grand canonical and micro canonical ensembles with corresponding distribution laws (using Lagranges method of undetermined multipliers). **[14 Hours]**

UNIT - II

Classical Thermodynamics:

Brief resume of concepts of laws of thermodynamics force energy, chemical potential and entropies. Partial molar properties – partial molar free energy, partial molar volume, partial molar heat content, their significance. Determination of these quantity concept of fugacity and its determine by graphical method and compressibility factor method. Non-ideal systems – excess functions for non-ideal solutions. Activity and activity co-efficient. Relationship between mole fraction, molality and molarity activity co-efficients. Determination of activity co-efficient by EMF and solubility methods, phase rule-derivation of phase rule from the concept of chemical potential, application of phase rule to three component systems. **[14 Hours]**

UNIT - III

Applications of Quantum Mechanics:

Application of variation theorem to a particle in one dimensional box, linear oscillators, H and He-atoms, SCF method for many electron atom. Slater orbitals – Effective nuclear charge (ENC), expressions for slater orbitals for 1s, 2s, 3s, 2p and 3d electrons (no derivation). Slater's rules for calculation of ENC – Slater's orbitals for He, Carbon and Nitrogen. Theories of valence – Introduction, linear and non-linear variation functions, secular equations, columbic, exchange, normalization and overlap integrals, secular determinants.

[14 Hours]

UNIT – IV

Solid State Chemistry:

Semi conductors – Bonding and conductivity, mechanism of conductivity, energy bands in semi-conductors, impurity conductors, p-n and n-p-n junctions. Importance of semiconductors. Super

conductors – occurrence of super conductivity, its destruction by magnetic fields, effect of IR and isotope effect, BCS theory of super conductivity, applications.
Defects in solids – Frenkel and Schotky defects and chemical reaction of solids. **[14 Hours]**

References:

1. Molecular thermodynamics – Donald A. Mc Quarrie, John D. Simon University Science Books, California, 1999.
2. Thermodynamics of Chemistry – S. Glastone, Affiliated East-West Press, New Delhi, 1960.
3. Statistical Thermodyanics – M.C. Gupta, Wiley Eastern Ltd., 1993.
4. Text Book of Physical Chemistry – Samuel Glastone, McMillan Indian Ltd., 2nd Edn. 1974.
5. Elements of Physical Chemistry – S. Glastone, McMillan Indian Ltd.,
6. Quantum Mechanics – L.I. Schiff, Pretice Hall, 1955.
7. Solid State Chemistry – C.N.R. Rao, Cambridge, CUP
8. Solid State Chemistry – N.B Hanna.

CSA SCT: 3.4: Applied analysis

56hrs

UNIT – I

Food analysis:

Objectives of food analysis. Sampling procedures. Detection and determination of sugars and starch. Methods for protein determination. Oils and fats and their analysis – iodine value, saponification value and acid value. Rancidity - detection and determination (peroxide number). Tests for common edible oils. Analysis of foods for minerals - phosphorus, sodium, potassium and calcium. General methods for the determination of moisture, crude fibre and ash contents of food. Analysis of milk for fat and added water. Non-alcoholic beverages -determination of chicory and caffeine in coffee; caffeine and tannin in tea. Alcoholic beverages -methanol in alcoholic drinks and chloral hydrate in toddy. Food additives - chemical, preservatives - inorganic preservatives - sulphur dioxide and sulphites, their detection and determination. Organic preservatives - benzoic acid and benzoates, their detection and determination. Flavouring agents - detection and determination of vanilla and vanillin. Coloring matters in foods - classification, certified colors, detection of water soluble dyes, color in citrus fruits, beet dye in tomato products, mineral color. Pesticide residues in foods - determination of chlorinated organic pesticides. Control food quality - codex alimentarius, Indian standards.

[14 Hours]

UNIT – II

Water pollution and analysis:

Water resources, origin of wastewater, types of water pollutants; their sources and effects, chemical analysis for water pollution control - objectives of analysis, parameters of analysis,

sample collection and preservation. Environmental and public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, chlorine demand, 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 and 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 and
tannin and lignin as water pollutants and their determination. **[14 Hours]**

UNIT III

Kinetic methods of analysis: Introduction, basis of kinetic methods, rate law expressions. Classifying chemical kinetic methods – direct-computation integral methods, direct-computation rate methods, curve-fitting methods. Instrumentation. Quantitative applications – enzyme catalyzed reactions, non-enzyme catalyzed reactions, non-catalytic reactions. Determining Vmax, Km for enzyme catalyzed reactions. Elucidating mechanism for the inhibition of enzyme catalysis. Determination of enzymes, LDH, GOT and GPT. Determination of substrates – urea, uric acid, blood glucose and blood alcohol. Analysis of closely related compounds - neglect of reaction of slow reacting component method and logarithmic extrapolation method.

Automated methods of analysis: An overview. Principles of automation. Automated instruments: process control. Continuous analyzers. Discrete autoanalyzers. Instruments used in automated process control. Automatic instruments - discrete and continuous flow sampling instruments. Flow injection analysis – principles - dispersion co-efficient. Factors affecting peak height, sample volume, channel length and flow rate, and channel geometry. Applications -limited dispersion applications, medium dispersion applications, stopped flow methods and flow injection titrations. Discrete automatic systems - centrifugal fast scan analyzer, automatic organic elemental analyzers.

Analysis based on multilayer films-general principles, film structures, instrumentation, performance and applications – blood urea nitrogen, blood glucose and potassium. **[14 Hours]**

UNIT IV

Biomedical and forensic analysis: Composition of body fluids and detection of abnormal levels of certain constituents leading to diagnosis of disease. Sample collection and preservation of physiological fluids. Analytical methods for the constituents of physiological fluids (blood, serum, urine). Blood - estimation of glucose, cholesterol, urea, haemoglobin and bilirubin. Urine - urea, uric acid, creatinine, calcium phosphate, sodium, potassium and chloride. 82Biological significance, analysis and assay of enzymes (pepsin, monoaminoxidase, tyrosinase); and hormones (progesterone, oxytocin, insulin). Chemical, instrumental and biological assays to be discussed wherever necessary.

Forensic analysis: General discussion of poisons with special reference to mode of action of cyanide, organophosphates and snake venom. Estimation of poisonous materials such as lead, mercury and arsenic in biological materials. **[14 Hours]**

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th

edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc. India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Instrumental Methods of Analysis by H.H. Willard, L.L. Merritt and J.A. Dean, 7th edition, (1988).
7. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.
8. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
9. Introduction to Instrumental Analysis, Braun, Pharm. Med. Press. India.
10. Instrumental Method of Analysis, W. M. Dean and Settle, 7th edition, 1986, CBS Publishers, New Delhi.
11. Instant Notes of Analytical Chemistry, Kealey and Haines, Viva books Pvt. Ltd., 2002.
12. Soil Chemical Analysis, M.L. Jackson, Prentice Hall of India Pvt. Ltd., New Delhi, 1973.
13. Clinical Chemistry, Principles and Procedures, J.S. Annino, 2nd edition, Boston: Little, Brown, 1960.
14. Methods of Geochemical Analysis, D. Click, Ed., A Multi volume series, NewYork, Inter science.
15. Clinical Chemistry, Principles and Techniques, R.J. Henry, D.C. Cannon and J.W. Winkleman, Eds., 2nd edition, Hagerstorm, M.D: Harper and Row, 1974.
16. Fundamentals of Clinical Chemistry, N.W. Tietz, Ed., 2nd edition, Philaddphia: W.B. Saunders, 1976.
17. Food Analysis, A.G. Woodman, McGraw Hill. 1971.
18. Chemical Analysis of Foods, H.E. Cox and Pearson.
19. Analysis of Foods and Food Products, J.B. Jacob.
20. A First Course in Food Analysis, A.Y. Sathe, New Age Internationals (P) Ltd., Publishers, Bangalore, 1999.

CSE SCT: 3.5: Environmental and Biochemical analysis

56 Hrs

UNIT – I

Environmental Segments, Air Pollution and Soil Pollution:

Air pollutants, prevention and control, Green house effect and acid rain. CO – industrial and transportation sources. So_x- sources, ambient concentration, test methods, control techniques – scrubbing, limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. NO_x – sources, ambient concentration, test methods, thermodynamics and NO_x, control techniques. Particulates: size distribution. Bhopal gas tragedy. Noise pollution.

Composition of soil – Inorganic and organic components in soil, micro and macro nutrients, nitrogen and sulfur pathways.

Soil pollution:

Classification of pollutants and their characteristics, sources, prevention and control. **[14 Hours]**

UNIT – II

Hydrologic cycle, sources, criteria and standards of water quality:

Safe drinking water, public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Determination of BOD, COD and TOC.

Toxic chemicals in the environment, impact of toxic chemicals on enzymes. Detergents – pollution aspects, Pesticides – pollution of surface water. Heavy metal pollution. Chemical speciation – biochemical effects of heavy metals (Hg, As, Pb, Se), carbon monoxide, nitrogen oxides, sulphur oxides and hydrocarbon. Treatment of industrial liquid wastes.

[14 Hours]

UNIT – III

Soil Analysis:

Physical properties of soils – soil texture and soil structure. Chemical properties of soil – types of soil collides, types of clays and their swelling and adsorption properties, cation exchange capacity and its determination, acid soils – types of soil acidity, liming, measurement of pH and conductivity of soil – saline and alkaline soils, analysis of major constituents of soil – organic matter, nitrogen, sulphur, potassium and calcium.

Fuel Analysis:

Solid, liquid and gaseous fuels; ultimate and proximate analysis, heating values, grading of coal; liquid fuels; flash point, anline point, octane number and cetane number, carbon residue; gaseous fuels; producer gas and water gas, calorific valves. **[14 Hours]**

UNIT – IV

Food Analysis:

Estimation of moisture, ash, crude protein, fat, crude fiber, carbohydrate, calcium, potassium, sodium and phosphate in foods; Analysis of common adulterants in food; Milk and milk products – alcohol test, fermentation test, dye reduction tests (methylene blue and resazurin), tests to distinguish butter and margarine, phosphate test for pasteurization, estimation of added water; Beverages – caffeine and chicory in coffee, methanol in alcoholic drinks; estimation of saccharin, coal tar dyes, aflatoxins in foods; pesticide analysis in food products – extraction and purification of sample, gas chromatography for organophosphates, thin-layer chromatography for chlorinated pesticides. **[14 Hours]**

References:

1. Principles of Instrumental Analysis, Skoog, Holler and Nieman, Harcourt Afca, 2001.
2. Environmental Chemistry – A.K. De, (Wiley Eastern).
3. Environmental Chemistry – S.K. Banerji, (Prentice Hall India), 1993.
4. Chemistry of Water Treatment – S. D. Faust and O. M. Aly, (Butterworths), 1983.
5. Environmental Chemistry – I. Williams, John Wiley, 2001.
6. Food Analysis – A. G. Woodman, McGrawHill, 1971.
7. Foods: Facts and Principles – Shadaksharaswamy and Manay, Wiley Eastern, 1987.
8. A Text Book of Soil Chemical Analysis – P. R. Hesse, CBS Publishers, 1994.

CHI HCP: 3.6 – Inorganic Chemistry

Preparation of Metal Complexes (any five):

1. Mercury tetrathiocyanatocobaltate(III).
2. Chloropentammine cobalt (III) chloride.
3. Nickel (II) salicylaldoxime.
4. Copper (II) acetyl acetone.
5. Tris thiourea copper (I) sulphate complex.
6. Hexammine cobalt (III) chloride.
7. Potassium bisoxalato cuprate (II) dihydrate.
8. Potassium trisoxalatoferrate (III).
9. Nickel (II) Schiff's base complex.

REFERENCES

1. A text book of quantitative inorganic analysis- A.I.Vogel, 3rd edition.
2. Vogel's text book of quantitative chemical analysis – J.Basset, R.C.Denney, G. H. Jeffere and J. Mendhom, 5th edition.
3. Quantitative chemical analysis – Daniel, C.Harris, 7th edition 2006.

CHI HCP: 3.7 – Organic Chemistry

Estimation of Organic functional Groups (Any Six)

1. Estimation of Hydroxyl Group (Alcohols and Phenols)
2. Estimation of Acetyl Group (O-acetyl)
3. Estimation of Methoxyl Group –Zeisel's Method
4. Estimation of carboxyl group
5. Estimation of Esters
6. Estimation of Amines
7. Estimation of Amide Group
8. Estimation of Urea
9. Estimation of Nitro Group

References:

1. Advanced physicochemical experiments – J. Rose
2. A Text Book of Quantitative Inorganic Analysis – A.I. Vogel, 5th Edn.
3. Instrumental Analysis Manual – Modern Experiments for Laboratory – G.G. Guilbault and L.G. Hargis.
4. Quantitative Chemical Analysis – Daniel C. Harris, 7th Edn., 2006.
5. Comprehensive Practical Organic Chemistry- VK Ahluwalia, Renu Aggarwal

OPEN ELECTIVE/ CROSS BORDER
PAPER-I
(NON CHEMISTRY STUDENTS ONLY)
OET SCT: 3.1 Analytical and Organic Chemistry

28Hrs

Unit-I

Principles of Chromatography:
Distribution coefficient, modes of chromatography, selection of stationary and mobile phases, analyte development and elution. Chromatographic performance parameters-retention time and volume capacity factor, plate height and resolution.

Gas Liquid Chromatography:
Principle, apparatus, columns, simple application, mobile phase, stationary phases, detectors, applications.

HPLC Principles:
Instrumentation –columns, stationary phase and matrices, simple application, mobile phase, pumps, detectors.

Ion-exchange Chromatography: Principle, material and applications.

Thin Layer Chromatography:
Principles, apparatus, preparations of plates, simple applications, plate development, detection of analytes. selection of chromatographic systems. [**14 Hrs]**

Unit-II

Organic Chemistry:
Introduction, classification of organic compounds with examples, classification of organic reactions with examples.

Nomenclature of Organic Compounds: IUPAC name of simple organic compounds.

Structure and Reactivity:
Acids and bases, structural effects on acidity and basicity, hydrogen bonding, resonance, inductive effect and hyperconjugation. Application of Huckel's rule to simple organic molecules.

Insecticides: Introduction, classification, mode of action of chlorinated insecticides, synthesis of DDT, malathion and beygon. **[14 hrs]**

REFERENCE

1. Modern analytical chemistry-David Harvey, Mc Graw Hill, New Delhi, 2000.
2. Fundamentals of analytical chemistry-D.A Skoog, D.M West, Holler and Crouch,8th edition, Sunder College Publishing, New York, 2005.
3. Analytical chemistry-G.D.Christian,5th edition John Willey and Son's, Inc., India,2001.
4. Organic chemistry-I.M.Morrison and Boyd.
5. Advanced organic chemistry-Jerry March.
6. Organic chemistry-I.L.Finar, Vol.I &II.

PAPER-II

OET SCT: 3.2 Quality Control, Assurance and Chromatographic Techniques

28 Hrs

UNIT-I

Quality Control and Assurance:

Role, government standards like ISI, MINAS, Agmark, I.P, D.P, U.S.P, ASTM and FMTM, concepts of quality and quality control , the nature of variability. Specification and tolerances, sampling inspection, cost reduction and quality improvement experiments, optimization.

Basic concepts of quality assurance, quality acceptance, sampling reliability, cost aspects of quality decisions. Quality control in raw materials, production and finished product. Current trends in quality control, ISO 9000 and ISO 14000 series. Laws related to quality control. ISO 17025.

Chemical Warfare Convention:

Definition and schedules. Toxic chemicals, remote control system, tear gas, chemical weapons, ocean dumping of chemical weapons. **[14hrs]**

UNIT-II

Chromatographic Techniques:

Principles, classifications and theory of chromatographic separation.

Ion exchange chromatography:

Structures of resins, selectivity, capacity of resins, ion exchange equilibria, application-removeval of interfering ions, concentration and recovery of traces, anions and cations separation and application for separation of lanthanides and actinides. Techniques of column chromatography and size exclusion chromatography.

Paper chromatography: Theory and principle.

Gas chromatography:

Principles column detectors- TCD, FID, ECD and column efficiency, capacity factors, resolution. Practical aspects of GC-Hypernated techniques.

HPLC: Principles, equipments, column, detectors, choice of column, materials. **[14 hrs**]

REFERENCE

1. Analytical chemistry – G.D.Christian, 6th edition, John Willey, 2004.
2. Quantitative analysis, A.Day and A.L.Underwood, 5th edition,1998.
3. Principles of instrumental analysis-Skoog, Holler and Nie man, Harcourt Afca, 2001.
4. Instrumental methods of analysis-H.H.Williard, L.L.Merit and J.J.Dean, 7th edition, 1988.
5. Chemical process industries-Shreves and R.Norries, 3rd edition, Mc Graw Hill, 1967.
6. Statistical quality control, 2nd edition, Manohar Mahajan, 1995.
7. Chemical engineers hand book-Robort H. Perry, 8th edition, Mc Hill, 1995.

FOURTH SEMESTER CHEMISTRY
CHO HCT – 4.1 ADVANCED ORGANIC CHEMISTRY

56 Hrs

UNIT – I

Hormones:

Introduction, classification, sterols, sex hormones, androgens, oestrogens. Non-steroidal oestrogens, and their clinical applications. Synthesis and mode of action of hormones. Androsterones, testosterones, estrones, estradiol, estriol.

Synthesis and therapeutic applications of: non-steroidal hormones: diethylstilbestrol, hexestrol and dienestrol. Progestins: progesterone, norethynodrel and norethindrone.

[14 Hours]

UNIT – II

Stereoselective synthesis:

Stereoselectivity: Classification, terminology and principle of stereoselectivity, Strategy of stereoselective synthesis. Acyclic stereoselection. Enantioselective synthesis, diasteroselection in cyclic compounds. Catalytic hydrogenation, alkylation, stereoselective formation of double bond, stereoselective cyclization of polyenes. Protection and deprotection of functional groups.

Retrosynthesis:

Introduction, retrosynthetic stragegies for target molecules: group oriented strategies, functional group interconversion (FGI), functional group addition (FGA), functional group removal.

Disconnection approach: Disconnection of bonds in ring systems and bonds joining ring atoms to functional groups or other residues. Retro Diels-Alder reaction. **[14 Hours]**

UNIT – III

Photochemistry:

Interaction of electromagnetic radiation with matter, types of excitations, Jablonski diagram, fate of excited molecule, quantum yield, transfer of excited energy.

Intramolecular reactions of the olefinic bond – Geometrical isomerism, cyclisation reactions, rearrangement of 1,4 – and 1,5 – dienes. Intramolecular reactions of carbonyl compounds – Saturated, cyclic and acyclic. α, β unsaturated compounds, Norrish type I and II reactions and photochemistry of cyclohexadienones. Intermolecular cycloaddition reactions – Dimerisations and oxetane formation. Patterno Buchi Reaction) Isomerisation, addition and substitutions of aromatic systems. **[14 Hours]**

UNIT – IV

Heterocyclic Chemistry – II

Transformations, Photochemistry and Rearrangement in Heterocycles.

Transformations:
i) Coumarins to benzofurans
ii) Sydonones to Pyrazoles
iii) Chromones to Pyrazoles
iv) Furans to Pyridines.
v) Pyrroles to Pyridines.

Heterocycles in Functional Group Transformations:
i) Alkanes from Thiophenes.
ii) Cycloalkanes from Pyrazolines.

iii) Dienes from Pyrroles.
iv) Alcohols from isoxazodiolines.
iv) Esters from Trichlorocyanuric acid
v) Acetylenes from 1,2,3-selenadiazoles and
vi) Deoxygenation of Phenols tetrazoles

Rearrangements in Heterocycles:

i) Dimoroth Rearrangement
ii) Boultan-Katritzky Rearrangement.
iii) Fischer Indole cyclisation. **[14 Hours]**

REFERENCES:

1. Fundamentals of photochemistry, K.K. Rohtagi Mukhjerji, Wiley – Eastern
2. Organic photochemistry, J. Coxon and B. Halton, Cambridge University, Press.
3. Molecular photochemistry, N.J. Turro, W. A. Benzamin.
4. Introductory photochemistry, A. Cox and T. Camp, McGraw Hill.
5. Molecular reactions and photochemistry, Depuy and Chapman.
6. Stereochemistry, conformation and mechanism – P. S. Kalsi
7. Stereochemistry of carbon compounds – E.L. Eliel
8. Stereochemistry of organic compounds – D. Nasipuri
9. Designing organic synthesis – S. Warren, Wiley.
10. Medicinal chemistry – Vol.I, II, and III – Burger
11. Text book of organic pharmaceutical chemistry – Wilson and Gisvold.
12. Bentley text book of pharmaceuticals – B.A. Rawlins
13. The organic chemistry of drug design and drug action – R. B. Silverman
14. An introduction to drug design – S. S. Panday and J.R. Dimmonds
15. Organic and pharmaceutical chemistry, Ed. Robert E. Dorge
16. An Introduction of the Chemistry of Heterocyclic Compounds – R.M. Achenson, 4th Edn., John Wiley & Sons.
17. Heterocyclic Chemistry – A.R. Katritzky and J.J. Logowskii.
18. Heterocyclic Chemistry – R.K. Bansal, 3rd Edn., New Age International Publishers (2002)

CHI HCT: 4.2 - Advanced Inorganic Chemistry (Bio-inorganic and Organometallic Chemistry)

56 Hrs

Bio-inorganic Chemistry:

UNIT – I

Metal Ions in Biological Systems:

Essential and types metals, active transport of Na and K, ionophores, metalloproteins as enzymes – carboxy peptidase, (catalases, peroxidases, cytochorome P450, copper oxidases), vitamin B_{12} coenzyme, enzyme action inhibition and poisoning. Synthetic model compounds. Metals in medicine – Metal deficiency (Fe, Mn, Cu and Zn), chelation therapy and metal complexes as drugs. **[14 Hours]**

UNIT – II

Heme and Non-heme Systems:

Chlorophyll and its role in photosynthesis, transport and storage of dioxygen – heme proteins, oxygen uptake, functions of haemoglobin, myoglobin, hemerythrin, and hemocyanins, synthetic oxygen carriers, metal storage and transport – ferritin and transferrin, Electron transfer proteins – cytochromes and iron sulphur proteins. Biological nitrogen fixation, in-vivo and in-vitro nitrogen fixation. **[14 Hours]**

Organometallic Chemistry

UNIT – III

Classification & nomenclature of organometallic compounds – 16 & 18 electron rules – electron counting by neutral atom & oxidation state method.

Organometallic compounds of main group elements:- General methods of synthesis structure & bonding in allkyls of Li, Mg, & Al. TM alkyls(synthesis and stability),metal carbonyls, nitrosyls, carbenes, Fischer and Shock synthesis and bonding.

General methods of synthesis, structure & bonding in metal olefins, metal carbonyls and metallocenes. **[14 Hours]**

UNIT – IV

Organometallic Reaction mechanisms and catalysis:

Fundamental reactions, substitution in carbonyl complexes, Mechanisms, Insertion reactions, CO, SO_2, olefin insertions, oxidative additions, one electron, addition of oxygen, reductive elimination, CH activation, Use of Organometallic Compounds as catalysts – Catalytic behaviour – Homo catalysis –. Anchoring of Catalysts. Use of organometallic compounds in the synthesis of organic compounds.

Hydrogenation. Hydrogenation of olefins (oxo reaction-cobalt and rhodium oxo catalysts), carbonylation of alcohols – Monsanto acetic acid process, Wacker process.

Polymerization of olefins and acetylenes: Ziiegler – Natta catalysis systems.

Fischer – Tropsch reaction, Water Gas Shift reactions. **[14 Hours]**

REFERENCES:

1. The Inorganic Chemistry of Biological process – M.N. Hughes, 2nd Edn. John Wiley and sons, 1988.
2. Bioinorganic Chemistry – R.N. Hay, Ellis Horwood Ltd., 1984.
3. Biological Inorganic Chemistry – An Introduction, R.R. Crichton, Elsevier, 2008.
4. Transition Metal Compress as Drugs and Chemothe – Rapentic Agents – N. Farrel Kluwer Academic Publication, 1989.
5. Inorganic Chemistry – I.E. Huheg, R.L. Keiter and A.L. Keiter, 4th Edn, Addison Wesley, 2000
6. Bioinorganic Chemistry – A.K. Das, Books & Allied (P) Ltd., 2007.
7. Organometallic Chemistry – R.C. Mehrothra and A. Singh, 2nd Edn., New Age, International Publications, 2006.
8. Fundamental Transition Metal Organometallic Chemistry – Charles M Lukehart, Brookes, Govel Publishing Company, 1985

9. The Organometallic Chemistry of the Transition metals: Robert H. Crabtree, 4th Edn., Wiley Interscience, 2005.
10. Basic Organ Metallic Chemistry – B.D. Gupta and A.J. Elias, Universities Press, 2010.
11. M.N. Hughes: Inorganic Chemistry of Biological Processes (2nd Edn.) Wiley
12. I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine: Bioinorganic Chemistry, Viva Books.
13. R.C. Mehrotra ad A. Singh: Organometallic Chemistry, New Age International.
14. F.A. Cotton and G. Wilkinson: Advanced Inorganic Chemistry, Wiley.
15. Concepts and Models of Inorganic Chemistry, Douglas, McDaniel, Alexander, 3rd Ed., Wiley India, 2012.

CHS_2, HCT: 4.3 Spectroscopy – II

56 Hrs

UNIT – I

Infra Red Spectroscopy

Introduction – Molecular vibrations – Mode of Vibrations, calculation of vibrational frequencies, Sampling techniques, interpretation of IR spectra factors affecting group frequencies and band shapes – Physical state of samples vibrational coupling, electrical and inductive effects, Hydrogen bonding and ring structures, co-relation chart, important regions in the IR spectrum – H stretching, triple bond, double band stretching, finger print region, applications of IR spectroscopy in the structural elucidation of organic. Compounds, application of far IR spectroscopy – Limitations of IR spectroscopy. (Problems & Exercise). IR spectraof coordination modes of ligands like nitrate, thiocynate, sulphate, carbonate(bridging, bidentate etc.,),aquo complexes. **[14 Hours]**

UNIT – II

HNMR Spectroscopy

Introduction – Nuclear spin and magnetic moment, origin of NMR spectra, Theory of NMR spectroscopy, resonance flipping, instrumentation and sampling, inter preparation of NMR spectrum, equivalent and non-equivalent protons, chemical shifts, stretching and destretching (down field and up field), factors influencing chemical shifts, anisotropic effects, NMR scale, units, internal references, simple and complex splitting / coupling, coupling constant, correlation chart of chemical shifts, spin-spin relaxations, deuterium exchange techniques limitations of H NMR spectroscopy – Introduction and applications of C^{13}NMR spectroscopy, 2 DNMR spectroscopy, use of PMR spectrum in structural elucidation of organic compound. ^{31}P and ^{10}F NMR spectra of simple organic molecules, phosphates, polyphosphates, PH_3, phosphohalides, fluoro acetic acid, SF_4, P_4S_4, HPF_2.

[14 Hours]

UNIT – III

Gas Liquid Chromatography:

Principle, apparatus-columns, sample application, mobile phase, stationary phase, detectors, applications.

HPLC Principles:

Instrumentation-columns, stationary phase and matrices, sample application, mobile phases, pumps, detectors

Mass Spectroscopy:

Introduction – Basic theory, ionsation, types of ions – molecular ion, fragment ion, meta stable ion, base peak, instrumentation, factors affecting fragmentation, intensity of M^+ peaks of alkanes, alkenes, alkynes, alcohols, amines, aldehydes and other compounds, Mc Laffarty rearrangement nitrogen rule, some simple examples of fragmentations, applications of mass spectrometry. GC-MS and LC-MS. **[14 Hours]**

UNIT – IV

Electron Spin Resonance Spectroscopy:

Introduction - Presentation of spectrum – ESR transitions and selection rules Hyperfine splitting in various structures – Factors affecting "g" values. Zero field splitting and Kramer's degeneracy Anisotropy in Hyperfine coupling constant – Nuclear Quadrupole interactions – Spin Hamiltonian – Electron delocalization instrumentations and applications

Mössbauer Spectroscopy

Introduction – Mössbauer effect – Resonance absorption of gamma rays conditions for Mössbauer spectroscopy – Mössbauer parameters – Isomer shift – electric quadruple interaction – Magnetic interactions – Instrumentation & applications to $Fe_3(CO)_{12}$, Prussian blue, Oxyhemerythrin, Hexacyano ferrates, Netroprusside and Tin halides.

Nuclear Quadruple Resonance Spectroscopy:

Introduction – Nuclear Quadruple Moment – Electric field gradient – Asymmetry parameter – Nuclear Quadruple transition – Effect of external magnetic field – Applications.

[14 hrs]

REFERENCES:

1. Spectroscopy of Organic compounds – P.S. Kalsi, Wiley Eastern Ltd. (India) / New Age International Publications, New Delhi (4th Edn.)
2. Organic Spectroscopy – William Kemp 3rd Edn. ELBS
3. Application of obsorption spectroscopy of organic compound – John R Dyer, Prentice Horll India, EEE, Recent Edn.
4. Instrumentation Method of Chemical analysis – G.R. Chatwal and S.K. Anand, Himalaya Publication House, Delhi (Recent Edn.)
5. Instrumentation method of chemical analysis. – B.K. Sharma – Goel Publishing House – Meerut.
6. Molecular structures and Spectroscopy – G. Aruldas, Prentice Hall India, New Delhi.
7. Spectroscopic methods in organic chemistry – D.H. Williams, I. Fleming – Tata McGraw Hill.
8. Introduction to NMR Spectroscopy – R.J. Abraham, J. Fisher, P. Loftus, - Wiley Publications.
9. Spectroscopic Identification of Organic Compounds – R.M. Silverstein, G.O. Basster and T.C. Morril – John Wiley Publication.

CHI SCT: 4.4 – Polymer Science and Technology

56 Hrs

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 in homogenous and heterogeneous systems, Polymerization Techniques. **Polydispersion-average molecular weight concept**.

Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance 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 testing-tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance. **[14 Hours]**

UNIT- II

Morphology and order in crystalline polymers - configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting poit Tm-melting points of homogenous 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 requirements and polymer utilization.

[14 Hours]

UNIT- III

Testing of Polymers: Need for testing-specifications and standards, mechanical-short term (tensile, fluxural, impact, tear resistance, abrasion resistance etc.,) long term (creep and fitigue). Electrical-conductivity, volume resistivity, surface, breakdown voltage, dielectric constant, loss factor, thermal coefficient of thermal expnasion, heat distortion temperature, vicat softening point, low temperature, properties, thermal conductivity.

Solution properties of polymers:

Polymer dissolution, criteria, thermodynamics, Floury-Huggins theory, nature of polymer molecules in solution, their size and shape, theta solvent, theta temperature, thermodynamics of mixing, solution viscosities. **[14 Hours]**

UNIT- IV

Polymer processing:

Plastics, electomers and fibres, compounding. Processing techniques; calendaring, die casting, rotational casting, film casting, injection molding, blow molding extrusion molding, thermoforming, foaming reinforcing and fiber spinning.

Properties of commercial polymers: Polyethylene, polyvinyl chloride, polyamides, polyester, phenolic resins, epoxy resins and silicon polymers. Functional polymers- fire retarding polymers and electrically conduction polymers, Biomedical polymers: contact lens, dental polymers, artificial heart, kidney skin and blood cells. **[14 Hours]**

REFERENCES:

1. Text book of Polymer Science (3rd edition) F.W.Billmayer, A Wiley-Interscience, 1984
2. Contemporary Polymer Chemistry (2nd edition), H.R.Allcock and F.W.Lampe, Prentice Hall, Englewood Cliff's, NewJersy 1981
3. Polymer Science, V.R.Gowswamy424784ariker, N.V.Viswanathan and Jayadev Sreedhar, New Age International (P) Limited, August 1996.
4. Introductory Polymer Chemistry, G.S.Misra, Wiley Eastern Limited, 1993
5. Polymer Science and Technology of Plastics and Rubbers, Premamoy Ghosh, Tata McGraw Hill, 1990
6. Polymer characterisation, Physical Techniques, D.Campbell and J.R. White, Chaopman and Hall, 1989.
7. Principles of Polymer Science Systems, F.Rodriguez, McGraw Hill Book co., 1970.

CSA SCT: 4.5- ADVANCED SELECTED TOPICS IN CHEMISTRY

56 Hrs

UNIT – I

Principles & concept of green chemistry

Introduction –Concept and Principles-development of Green Chemistry- Atom economy reactions – Selection of starting materials, Designing biodegradable products, Green reaction conditions, Green catalysis, Ionic liquids, Supercritical fluids, Flourous phase reactions, Heterogeneous catalysis: Biocatalysis: -toxicity measures- Need of Green Chemistry in our day to day life.

Renewable resources

Biomass –Renewable energy – Fossil fuels-Energy from Biomass-Solar Power- Other forms of renewable energy-Fuel Cells-Alternative economics-Syngas economy- hydrogen economy-Bio refinery chemicals from fatty acids-Polymer from Renewable Resources –Some other natural chemical resources. **[14 Hours]**

UNIT – II

Measuring and controlling environmental performance

Importance of measurement – lactic acid production-safer Gasoline – introduction to life cycle assessment-four stages of Life Cycle Assessment (LCA) –Carbon foot printing-green process, Matrics-eco labels -Integrated Pollution and Prevention and Control(IPPC)-REACH (Registration, Evaluation, Authorization of Chemicals)

Emerging green technology and alternative energy sources

Design for Energy efficiency-Photochemical reactions- Advantages-Challenge faced by photochemical process. Microwave technology on Chemistry- Microwave heating –Microwave assisted reactions-Sono chemistry and Green Chemistry –Electrochemical Synthesis-Examples of Electrochemical synthesis. **[14 Hours]**

UNIT – III

Supramolecular chemistry

Supramolecular Chemistry, Classification, Thermodynamic and Kinetic selectivity, Supramolecular interactions,

Supramolecular host design, Macrocyclic versus acyclic hosts, High dilution synthesis,Template synthesis, Cation binding, cryptaspherands, heterocrowns, hetero-cryptands, selectivity of cation complexation, anion binding hosts, concepts in anion host design, cation hosts to anion hosts, pH effect, Self assembly-basic concepts, Template effect on self assembly, Kinetic and Thermodynamic considerations, Self assembly of coordination complexes. Solid state supramolecular chemistry, Supramolecular Photochemistry. **[14 Hours]**

UNIT – IV

CHEMISTRY OF NANOMATERIALS

Introduction: Scope and importance of nanoscience and nanotechnology. Synthetic Methods: Chemical Routes : Physical methods, Techniques for characterization:, BET method for surface area analysis, dynamic light scattering for particle size determination. Studies of Nano-structured Materials: Synthesis, properties and applications of the following nanomaterials, fullerenes, carbon nanotubes, core-shell nanoparticles, self- assembled monolayers, nanocrystalline materials, magnetic nanoparticles thermoelectric materials, non-linear optical materials, liquid crystals. **[14 Hours]**

References:

1. T. Pradeep, NANO: The Essentials, McGraw-Hill, 2007.
2. B S Murty, P Shankar, Baldev Rai, BB Rath and James Murday, Textbook of Nanoscience And Nanotechnology, Univ. Press, 2012.
3. V. K. Ahluwalia, M. Kidwai, New trends in Green Chemistry, New Age Publications, 2004.
4. P.T. Anastas and J.C. Warner, Green Chemistry, Theory and Practice, Oxford University Press, 2000.
5. Jonathan W. Steed, David R. Turner, Karl J. Wallace, Core Concepts in Supramolecular Chemistry and Nanochemistry, John Wiley & Sons, 2007.
6. Jonathan W. Steed, Jerry. L. Atwood, Supramolecular Chemistry, John Wiley & Sons, 2002
7. Alfred Burger, Donald J. Abraham, Burger's Medicinal Chemistry and Drug Discovery: Chemotherapeutic Agents, 6th Edition, Wiley Inter Science, 2003.
8. N. K. Jain, Advances in Controlled and Novel Drug Delivery, CBS, 2001.
9. Mike Lancaster , Green Chemistry and Introductory text, II Edition
10. P.T.Anastas and J.C Warner,Green Chemistry theory and Practice, Oxford University press, Oxford (1988).
11. P.Tundo*et. al.*, Green Chemistry, Wiley –Blackwell, London (2007).
12. Protti D.Dondi *et.al.,*Green Chemistry
13. T.E Graedel, Streamlined Life cycle Assessment, Prentice Hall, NewJersey (1998).
14. V.K. Ahluwalia,Methods and Reagents of Green Chemistry: An Introduction by Green Chemistry. www.clri.org

CHP: HCP: 4.6- PROJECT WORK