GOVERNMENT COLLEGE FOR WOMEN (AUTONOMOUS)
KUMBAKONAM
DEPARTMENT OF CHEMISTRY
PG REVISED COURSE STRUCTURE UNDER CBCS
(For the candidates admitted from the academic year 2018-19)

SEMESTER –I

Sem	Course structure	Course code	Title of the paper	INS. Hrs /week	CREDIT	Exam hours	Marks		Total
							Int	Ext	
I	Core course I (CC)	P18CHC101	Inorganic chemistry – I	**6**	**5**	**3**	**25**	**75**	**100**
	Core course II (CC)	P18CHC102	Physical chemistry – I	**6**	**5**	**3**	**25**	**75**	**100**
	Core course III(CC)	P18CHC103P1	Inorganic chemistry Practical – I	**6**	**4**	**6**	**40**	**60**	**100**
	Core course IV (CC)	P18CHC104P2	Organic chemistry Practical – I	**6**	**4**	**6**	**40**	**60**	**100**
	Elective Course (EC) I A	P18CHC1EC1:1	Organic chemistry	**6**	**5**	**3**	**25**	**75**	**100**
	I B	P18CHC1EC1:2	Solid state Chemistry						
	I C	P18CHC1EC1:3	Green Chemistry						
			Total	**30**	**23**				**500**

SEMESTER –II

Sem	Course structure	Course code	Title of the paper	INS. Hrs /week	CREDIT	Exam hours	Marks		Total
							Int	Ext	
II	Core course IV(CC)	P18CHC205	Inorganic chemistry – II	**6**	**5**	**3**	**25**	**75**	**100**
	Core course VI (CC)	P18CHC206	Organic chemistry – II	**6**	**5**	**3**	**25**	**75**	**100**
	Core course VII(CC)	P18CHC207P3	Inorganic chemistry Practical – II	**6**	**4**	**6**	**40**	**60**	**100**
	Core course VIII (CC)	P18CHC208P4	Organic chemistry Practical – II	**6**	**4**	**6**	**40**	**60**	**100**
	Elective Course (EC) II A	P18CH2EC2:1	Analytical chemistry	**6**	**5**	**3**	**25**	**75**	**100**
	II B	P18CH2EC2:2	Supra molecular Chemistry						
	II C	P18CH2EC2:3	Textile Chemistry						
			Total	**30**	**23**				**500**
NCGPA (Internship)		INT	INTERNSHIP	**30**	**2**	**-**	**-**	**-**	**-**

SEMESTER –III

Sem	Course structure	Course code	Title of the paper	INS. Hrs /week	CREDIT	Exam hours	Marks		Total
							Int	Ext	
III	Core course IX(CC)	P18CHC309	Inorganic chemistry – III	**6**	**5**	**3**	**25**	**75**	**100**
	Core course X(CC)	P18CHC310	Organic Spectroscopy	**6**	**5**	**3**	**25**	**75**	**100**
	Core course XI (CC)	P18CHC311	Physical chemistry - II	**6**	**5**	**3**	**40**	**60**	**100**
	Core course XII (CC)	P18CHC312P5	Physical chemistry Practical – I	**6**	**4**	**6**	**40**	**60**	**100**
	Elective Course (EC) III A	P18CHC3EC3:1	Medicinal chemistry	**6**	**5**	**3**	**25**	**75**	**100**
	III B	P18CHC3EC3:2	Bio Organic Chemistry						
	III C	P18CHC3EC3:3	Chemistry of Nano Science						
			Total	**30**	**24**				**500**

SEMESTER –IV

Sem	Course structure	Course code	Title of the paper	INS. Hrs /week	CREDIT	Exam hours	Marks		Total
							Int	Ext	
IV	Core course XIII(CC)	P18CHC413	Physical chemistry - III	**6**	**5**	**3**	**25**	**75**	**100**
	Core course XIV (CC)	P18CHC414P6	Physical chemistry Practical – II	**6**	**4**	**3**	**40**	**60**	**100**
	Core course XV (CC)	P18CHPW415	Project	**12**	**6**	**-**	**-**	**-**	**100**
	Elective Course (EC) IVA	P18CHCEC4:1	Recent trends in chemistry	**6**	**5**	**3**	**25**	**75**	**100**
	IV B	P18CHCEC4:2	Industrial Chemistry						
	IV C	P18CHCEC4:3	Experimental methods in Chemistry						
			Total	**30**	**20**				**400**
				120	**90**				**1900**

Core Course papers : 14

Elective course papers : 4

Project : 1

CORE COURSE I – INORGANIC CHEMISTRY– I

UNIT – I **(18 hours)**

Acids and Bases : Brownsted and Lewis acids and bases, pH, pKa, acid – base concept in non – aqueous media, buffer solution, Protonic Acids – Proton Affinities – Differentiating and leveling Solvents – Acidic behaviour of the Binary hydrides – Strength of oxyacids – Hydrolysis – Amphoteric oxides – Non protonic concepts of Acid – base Reactions – Lux concept. Classification of Acids and Bases as Hard or Soft – Acid – Base Strength and Hardness and softness – Symbiosis – Theoretical basis of Hardness and softness – Electronegativity and hardness and Softness. Non aqueous solvent – Liquid Ammonia, Acetic acid, bromine trifluoride, dinitrogen tetroxide, liquid hydrogen fluoride as solvents.

UNIT II **(18 hours)**

Ionic Bond Crystal structure and Advances Covalent Bonding :

Ionic bonding – definitions and example.

Lattice energy – Born Lande equation derivation – important points arising from Born Lande equation. Application of lattice energy – Radius Ratio rules – calculation of some limiting radius ratio values for CN.3 (planar triangle), CN.4 (tetrahedral), C.N.6 (octahedral).

Classification of Ionic Structure :

AX, AX_2, AX_3, types AX type (ZnS, NaCl, ad CaCl) structure only. AX_2 tyoe flupride, rutile, beta crystobalite (structure only). Layer structure – CdI_2, Nickel arsenide structures. Schottky defect and Frenkel defect – explanation and calculation of number of defects from cm^3 – metal excess defect – F Centers and interstitial ions – Metal deficiency defect – positive ions absent – extra interstitial negative ions – Band theory of solids – insulators, semiconductors, and superconductors.

UNIT III **(18 hours)**

Nuclear Chemistry :

Radioactive decay – Theories of decay processes – Laws of radioactivity – Detection and Measurements of radiations – Nuclear structure – Composition of nuclei – properties of nuclei – nuclear radii – nuclear spin ect. – nuclear forces – its characteristics – Meson Field theory – nuclear stability – nuclear models – liquid drop, shell and collective models.

Artificial Radioacivity

Nuclear reactions – transmutation – Stripping and pick up, Fission product and fission yields, fusion, spallation and fragmentation reactions scattering reactions – nuclear cross section – Q – value nuclear reactors – charged particle accelerators.

Radioactive techniques – tracer technique neutron activation and isotopic dilution analysis, counting techniques such as G.M. ionization and proportional counter.

Applications of nuclear science in agriculture and biology.

Radiation risks and medical benefits – Natural and manmade isotopes.

UNIT IV **(18 hours)**

Polyacids anions :

Basic building, units of vanadate, molybdate and tungstate ions – apex sharing structure only Heterpoly anions – structure only.

Inorganic polymers :

Rings, Phosphazenes – structure – Craig and paddock model – Dewar model Cages of phosphorus – Boron hydrides and carboranes.

Clusters :

Metal clusters, dinuclear clusters – structure of Re_2Cl_8 – Qualitative M.O. diagrams for dinuclear rhenium and molybdenum complexes to explain the strength of quadrapole bond.

UNIT V **(18 hours)**

Chemistry of metals and Rare gases :

General properties of metals, occurrence, principles of isolation and complex formation of s,p and d block metals. Chemistry of lanthanides and actinides – Spectral and Magnetic properties, lanthanide contraction.

Rare gas : Isolation Chemistry and structure of rare gas compounds (Xenon Compounds)

References :

1. Badie E. Duglas and Danl H.M. Daniel. Concepts and Models in Inorganic chemistry, Indian Edition, 1970, Oxford and IBH Publishing co., New Delhi.
2. J.D.Lee, A New concise Inorganic chemistry 4th Edition, ELBS, 1995 (UNIT – II)
3. G. Friedlander, J.W.Kennady and J.M.Miller, Nuclear and Radiochemistry (UNIT – III)
4. Keith F. Purchell and John, C.Ktz Inorganic chemistry, Saunders Golden Sunburst series W.B. Saunders Company Philadelphia.
5. Cotton and Wilkinson, Advances Inorganic Chemistry 5th edition, john Wiley and sons Newyork (UNIT IV)
6. W. Kain and B.Schwederski, bioinorganic chemistry, Inorganic elements in the Chemistry of life, John Wiley and Sons, Newyork (UNIT V)
7. James E. Huheey, Ellen A, Keiter and Richard L. Keiter, Inorganic Chenistry; principles of structure and reactivity, 4th Edition, Addison – Wesley Newyork, (UNIT I)
8. Shriver and Atkins, Inorganic chemistry, III Edition Oxford, 1999. India Gopssons PVT Ltd A – 14 Sector Noida.
9. Nuclear Physics by Arumugam
10. Inorganic chemistry by Sathya Prakash

CORE COURSE II – PHYSICAL CHEMISTRY – I

UNIT I **(18 hours)**

Quantum Chemistry – I : Schrodinger wave equation – elementary ideas on time dependent SWE – postulates of quantum mechanics – operator algebra – linear, non – linear, ladder, Hermitian operators (definition and theorms) – eigenfunctions and eigenvalues, normalization orthogonality – principle of superposition.
Application of SWE to model systems – particles in one and three dimenstional boxes – quantum numbers – distortion of the box, zero point energy and uncertainity principles – finite potential energy barriers and tunneling (definition only)

UNIT II **(18 hours)**

Molecular Spectroscopy : I Introduction aspects – interaction of radition with molecules – Einstein coefficient of absorption and transtition probabilities – basics of selection rules representationof spectra – the width and intensity of spectral transition – oscillator of strength.
Electronic Spectra : Electronic spectra of molecules - Born Oppenheimer approximation vibrational course structure - Frank - Condon principle – dissociation energy - rotational fine structure of electronic vibrational transtitions – Fortrate diagram.
Pre – dissociation – symmetry selection rules – polarization of bonds – various types of transtition – solvent effect on spectra. Photoelectron spectroscopy; basic principles – UPES, XPES and AES – Valence and Core binding analysis, koopman's theorm – ESCA and auger spectroscopy to the study of surfaces.

UNIT III **(18 hours)**

Classical Thermodynamics : Thermodynamics of systems of variable composition – partial molar quantities and additivity rules – chemical potential – relationship between partial molar quantities – Gibbs – Duhem equation – calculation of partial molar quantities from experimental data – Thermodynamis properties of real gases – fugacity – definition, calculation (real) and variation of fugacity temperature, pressure and composition (Duhem – Margules equation) – activity and activity co-efficient, definition – standard states – colligative properties and the activity of the solute – experimental determination of activity and activity coefficients of non electrolytes – activity in electrolytic solutions – determination of activity coefficient of electrolytes by freezing points.

UNIT IV **(18 hours)**

Chemical kinetics : Theories of reaction rates (bimolecular collision theory, absolute reaction rate theory (ARRT) – significance of reaction co – ordinate – molecular dynamics –

potential energy surfaces – kinetic isotopic effect – Lindemann's theory for unimolecular gaseous reactions.

Principles of microscopic reversibility – steady – state approximation chain reactions – thermal and photochemical reactions between hydrogen and halogen – gas phase auto oxidation, explosions and hydrogen – oxygen reactions. Factors influencing reaction rates in solutions – application of ARRT to solution kinetics – effect of solvents – double sphere and single sphere model and effect of ionic strength – influence of pressure on rates in solution – significance of volume of activation.

Homogeneous catalysis – acid base catalysis - Bronsted relation – Enzyme catalysis – mechanism of single substrate reactions – Michaelis Mentan law – influence of pH and temperature.

UNIT V

Fast reaction techniques(18 hours)

Flow methods (continuous and stopped flow methods) – Relaxation method (T and P jump methods) – Pulse techniques (pulse radiolysis, flash photolysis, shock tube method) – molecular beam method – lifetime method.

Photochemistry and Radiation chemistry

Photophysical processes in electronically excited molecules Jablonski diagram – Stern – Volmer equation and its applications – experimental techniques in photochemistry – chemical actinometers – laser and their applications.

Radiation chemistry : Differences between radiation chemistry and photochemistry – sources of high energy radiation and interaction with matter – radiolysis of water, solvated electrons – definition of G value – Curie – Linear energy transfer LET and Rad Scanvenging techniques – use of dosimetry and dosimeters in radiation chemistry – applications of radiation chemistry.

References:

1. A.K. Chandra, Introductory Quantum Chemistry, 4th ediion, Tata – MeGraw Hill, 1994.
2. R.K. Prasad, Quantum Chemisatry, 2nd Ed., New Age International Publishers 2000
3. I.N. Lenine, Quantum Chemistry 4th Ed., Prentice Hall of India Pvt. Ltd.
4. D.A.MeQuarrie, Quantum Chemistry, University Science Books 1998
5. P.W.Atkins, Molecular Quantum Mechanics, clarendon 1973
6. S. Glasstone, therodynamics for Chemists East – West Affilited Pvt Ltd., New Delhi.
7. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, Wiley Eastern Ltd.
8. M.G.Arora Nuclear Chemistry.
9. Arnicker, Nuclear Chemistry.
10. Glasstone, Source book on atomic energy.

CORE COURSE – III INORGANIC CHEMISTRY PRACTICAL – I

Titrimetry and Gravimetry

I.Estimation of mixture solutions

1. Cu (V) and Ni (G)
2. Cu (V) and Zn (G)
3. Fe (V) and Ni (G)
4. Zn (V) and Cu (G)

II. Preparation of compounds

1. Tetrammine copper (II) sulphate
2. Potassium trioxalato aluminate (III)
3. Tris thiourea copper (I) chloride
4. Tris thiourea copper (I) sulphate

CORE COURSE IV – ORGANIC CHEMISTRY PRACTICAL – I

I. Qualitative analysis of an organic mixture containing two components

Pilot separation, Bulk separation, Analysis, Derivatives.

II. Preparation of Organic compounds (Single stage)

1. Para-bromo acetanilide from acetanilide (bromination)
2. Para-nitro acetanilide from acetanilide (nitration)
3. 2,4,6-tribromo aniline from aniline (bromination)
4. Salicylic acid from methyl salicylate (Hydrolysis)

ELECTIVE COURSE I – ORGANIC CHEMISTRY I

UNIT I **(18 hours)**

Nomenclature of Organic compounds : - Naming of linear and branched alkanes, alkenes, polyenes and alkynes with and without functional groups by IUPAC nomenclature – aromatic and heteroaromatic system – nomenclature of heterocyclics having not more than one hetero stoms such as oxygen, nitrogen and sulphur – Nomenclature of alicyclic, bicyclic and tricyclic compounds.

Reactive intermediates : - Free radicals, carbenes, nitrenes, carbocation and carboanion – generation, stability, structure and reactivity – nonclassical carbocation.

Electronic effects : - Inductive effect – resonance effect – hyperconjugation (Baker Nathan effect) – hydrogen bonding – (inter and intra molecular)

UNIT II **(18 hours)**

Organic Stereochemistry – I : Principles of symmetry concepts of chirality – optical purity elements of symmetry and chirality – Newman, Sawhorse Fisher and flying wedge notations – Representation and interconversion – types of molecules exhibiting optical activity – Configurational nomenclature D and L & R and s nomenclature alicyclic and cyclic chiral compounds – stereo chemistry of allenes, spiranes (Atropisomerism) Stereochemistry of ansa compounds, cyclophanes and trans cyclic alkenes,

Definition of terms like prochirality, enantiotrophic and diastereotopic groups faces asymmetric sysnthesis – Cram's rule.

UNIT III **(18 hours)**

Organic stereochemistry – II : Geometrical isomerism : E and Z nomenclature determination of configuration of the geometrical isomers.

Configuarion of cyclic and bicyclc ring systems : Cis and trans nomenclature of three, four, five and six membered substituted cyclic systems – configuration of cyclohexane mono and di substituted cyclohexanes, decalins.

Dynamic stereochemistry : Quantitative relations between conformation and reactivity. Winstein – Eliel equation,Curtin – Hammett principle – Conformation reactivity and mechanism of cyclic systems – saponification of an ester, esterification of an alcohol, chromic acid oxidation of cyclohexanol – Stereospecific and stereoselective reactions.

UNIT IV **(18 hours)**

Methods of dertermining reaction mechanisms : Thermodynamic and kinetic aspects of organic reactions – energy profile diagrams – intermediate versus transition states, isotope effect– Product analysis and its importance – crossover experiments – isotopic labeling studies.

Correlation analysis : Linear free energy relation – Hammett equation – significance of sigma and rho applications. Taft, Swan, Scott, Grunwald – Winstein equation and their applications. Classification of solvents.

UNIT) V **(18 hours)**

Natural Products : Polysaccharides – structure of starch and cellulose configuration of carbohydrates – photosynthesis.

Peptides and proteins : Primary, secondary,tertiary and quaternary structures of proteins. Protection of N – terminal and C – terminal groups of proteins – synthesis of peptides. Merrifield solid state peptide synthesis.

Nucleic acids : chemistry of nucleic acids – structure of DNA properties biological implications of DNA, replication of DNA, structure of RNA – types of RNA and their functions. Determining the base sequence of DNA.

References:

1. J. March, " Advanced Organic Chemistry Reactions, Mechanisms and Structure", 4th edition, Wiley 1992.
2. R.K.Bansal "Organic reaction mechanisms" Tata McGraw Hill,1975.
3. P.S.Kalsi "Organic reaction mechanisms",New age international publishers.
4. E.L.Eliel "Stereochemistry of Organic compounds".
5. D.Nasipuri "Stereochemistry of Organic compounds".
6. I.L.Finar "Organic Chemistry" Vol. II, 5th edition ELBS, (1975)
7. O.P. Agarwal "Chemistryof Organic natural products" Vol. I&II
8. Chatwal "Chemistry of Organic natural products" Vol.

SOLID STATE CHEMISTRY

Theory Hours :6 **Exam Hours : 3**	**Course code : P20CHC3EC3** **Credits :4** **Marks : Max marks -100** **Ext - 75** **Int - 25**

OBJECTIVES

1. To learn the crystal structures of few inorganic solids.
2. To study the chemistry of crystallization and vapour phase transport.
3. To learn the applications of magnetic materials.
4. To study the chemistry of organic solids.

UNIT I: Crystal Structure and Crystal Engineering of Organic Solids

Types of close packing – hcp and ccp – packing efficiency – SC, BCC, and FCC, radius ratio rule – applications – polyhedral description of solids – structure types: Na2O, Cs2O, rutile, perovskite (ABO3), ReO3, K2NiF4, spinels and antispinels.

Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis – polymorphism and pseudopolymorphism – supramolecular isomorphism, polymorphism and crystal engineering of pharmaceutical phases.

UNIT II: Metallo Organic Frameworks

M.O.Fs (Metallo Organic Frameworks) – organometallic systems – combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. Design of nanoporous solids.

Interligand hydrogen bonds in metal complexes – implications for drug design – crystal engineering of NLO and OLED materials.

UNIT III: Preparative Methods in Solid State Chemistry

Experimental procedure, coprecipitation as a precursor to solid state reaction, other precursor methods, kinetics of solid state reactions – crystallizations of solutions, melts, glasses and gels, solutions and gels: zeolite synthesis – precipitation from solution or melt: flux method, epitaxial growth of thin layers, verneuil flame fusion method.

Graphite intercalation compounds, transition metal dichalcogenide and other intercalation compounds, ion exchange reaction, synthesis of new metastable phases by ‘Chimie Douce’.

Electrochemical reduction methods – preparation of thin films, chemical and electrochemical methods, physical methods – growth of single crystals, Czochralski method, Bridgman-Stockbarger methods – zone melting.

Vapour phase transport, hydrothermal methods, comparison of different methods – high pressure and hydrothermal methods and dry high pressure methods.

UNIT IV: Magnetic Materials and Optical Properties

Selected examples of magnetic materials and their properties – metals and alloys, transition metal oxides, spinels, garnets, ilmenite and perovskites.

Magnetoplumbites – applications – structure/property relations – transformer, information storage, magnetic bubble memory devices, permanent magnets.

Luminescence, Lasers and phosphors – definitions and general comments, configurational coordinate model, some phosphor materials, anti-Stokes phosphors – lasers – the ruby laser, Neodymium lasers

UNIT V: Organic Solid State Chemistry

Topochemical control of solid state organic reactions – intramolecular reactions – conformational effects – intermolecular reactions – molecular packing effects – photodimerization of 2-ethoxycinnamic acid (α form, β form, γ form) – photopolymerization of 2,5-distyrylpyrazine – photopolymerizations of diacetylenes.

Asymmetric syntheses – dimerization of anthracene – control of molecular packing arrangements.

Organic reactions within inorganic host structures – electrically conductive organic solids – organic metals, conjugated systems, doped polyacetylene, polyparaphenylene, polypyrrole – organic charge transfer complexes – new superconductors

REFERENCES

1. A. R. West, Solid State Chemistry and Its Applications; 2nd Ed., John Wiley and sons, New York, 2014 (Unit III – V).
2. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, 1995.
3. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, Amsterdam, 1989.
4. G. R. Desiraju, and T. Steiner, The Weak Hydrogen Bond in Structural Chemistry and Biology; Oxford University Press: Oxford, 2002.
5. G. A. Jeffrey, Introduction to Hydrogen Bonding; Oxford University Press, New York, 1997.
6. J. M. Lehn, Transition Metals in Supramolecular Chemistry; Vol 5, John Wiley and Sons, New York, 1999.
7. C. N. R. Rao, Current Science, 2001, 81, 1030.
8. Journals:

(i) Crystal Growth and Design.http://www.pubs.acs.org/journals/cgdefu/index.html

(ii) Crystal Engineering Communication, http://www.rsc.org /Publishing/ Journals /ce/ index.asp

SEMESTER - II
ELECTIVE COURSE – I (B)
GREEN CHEMISTRY

Theory Hours : 5	**Course code : P20CH2EC2**
Exam Hours : 3	**Credits :4**
	Marks : Max marks -100
	Ext - 75
	Int - 25

OBJECTIVES:

- To impart knowledge of green chemistry
- To learn about the techniques used in green chemistry for synthesis of various organic compounds.

UNIT I

Introduction to Green Chemistry

Introduction to green chemistry – twelve principles of green chemistry – planning a green synthesis in a chemical laboratory – evaluating the type of reaction involved –rearrangement, addition, substitution, elimination and pericyclic reactions. Selection of appropriate solvent – aqueous phase reaction – reactions in ionic liquids –organic synthesis in solid state – solid supported organic synthesis – selection of starting materials – use of protecting group – use of catalyst – use of microwaves and sonication.

UNIT II

Addition and Condensation Reactions

Addition reactions – Michael addition in aqueous medium and solid state – Diels-
Alder reactions in aqueous phase.Condensation reactions – Aldol condensation of aldehydes with nitroalkanes andnitriles – Aldol condensation in solid phase – benzoin condensation under catalyticconditions – applications.

UNIT III

Oxidation and Reduction Reactions

Oxidation reactions – Baeyer-Villiger oxidation in aqueous phase and solid state –
enzymatic Baeyer-Villiger oxidation. Reduction reactions – Clemmensen reduction – mechanism – limitations – applications

UNIT IV

Phase-Transfer Catalyst Reactions

Phase-transfer catalyst reactions – Heck reaction – Michael addition reaction –oxidation of toluene to benzoic acid – Reimer-Tiemann reaction – Baker-Venkataraman synthesis – Williamson ether synthesis – Dozen reaction.

UNIT – V

Sonication Reactions

Sonication reactions – Barbier reaction – Reformatsky reaction – Simmons-Smith
reaction – Strecker synthesis – Ullmann coupling reaction – Wurtz reaction –Bouveault reaction

REFERENCES

1. V. K. Ahluwalia, Green Chemistry; 2nd Ed., Ane Books Pvt Ltd., New Delhi, 2016. [UNIT- I, II, III, IV, V]
2. P. T. Anastas and J. C. Warner, Green chemistry Theory and Practice, Oxford University Press, New York, 2005. [Unit-I]
3. V. K. Ahluwalia and K. Agarwal, Organic Synthesis, Special Techniques, 2nd Ed., Narosa Publishing House, New Delhi, 2007. [Unit-I]

SEMESTER II

CORECOURSE – V INORGANIC CHEMISTRY – II

UNIT I **(18 hours)**

Co – ordination Chemistry :

Nomenclature of mono and polynuclear complexes – Crystal field theory – shapes of d orbitals in octahedral symmetry – CFSE strong field and weak field splitting – Calculation of CFSE for d 10 system. Splitting

in tetrahedral symmetry-only weakfield splitting.Jahn-Teller distortion,splitting pattern in trigonal, square planar, tetergonal, trigonal bipyramidal, square pyramide and cubic symmetries . Factors affecting the magnitude of spslitting (10Dq) – Spectrochemical series. Jorgensens relation. Evidences for CFT. Magnetism and color of transition metal ions, LFT.

M.O. Theory – Octahedral, tetrahedral and square planar complexes, pibonding and M.O. theory – ligand having empty and filled pi bonds – effect on 10Dq. Evidences for Pi bonding from X – Ray Crystallography, IR and Photoelectorn spectroscopy. Nephelauxtic effect.

UNIT II **(18 hours)**

Kinetics and mechanisms of reaction in solutions:

Labile and inert complexes, ligand displacement reactions – hydrolysis equation in octahedral and planar complexes – trans effect. Electron transfer reaction – Complementary and non complementary types – inner sphere and outer sphere processes – isomerization and racemization. Reaction of coordinated ligands, Template effect and synthesis macrocyclic ligands.

Stability of co – ordination compounds

Detection of complex formation in solution, Stability constants, stepwise and overall formation constants pH metric, polarographic and photometric methods of determining of formation of constants. Factors affecting stability – statistical and Chelate effects.

UNIT III **(18 hours)**

Inorganic photochemistry : Electronic transitions in metal complexes – metal centered and charged transfer reactions. Various photophysical and photochemical processes of coordination compounds – unimolecular charge – transfer photochemistry of Cobalt (III) complexes. Mechanism of CTTM photoreduction, ligand field photochemistry of Chromium (III) complexes. Adamson's rule. Photo active excited states, V-C model – photophysics and photochemistry of ruthenium – polypyridine complexes, emission and redox properties – photochemistry of organo metallic compounds, metal carbonyl compounds, compounds with metal – metal bonding. Reinecke's salt – chemical actinometer.

UNIT IV **(18 hours)**

Complexes of pi-acceptors ligands : Carbonyls – 18 electron rule – isolobal – applications to structure of carbonyl compounds (simple and poly nuclear) carbonylate anions, carbonyl hydrides,nitrosyl complexes – binding and terminal nitrosyl – bent and linear nitrosyl – dinitrogen complexes.

Metallocences – reactions – catalysis by organo metallic compounds. Hydrogenation and hydroforylation of olefins, aldehydes and ketones-polymerisation of alkenes cyclo-oligomerisation of acetylene-Fisher -Tropsch systhesis.

UNIT V **(18 hours)**

Bio – Inorganic Chemistry

The biological roles of metal ions, calcium biochemistry, oxygen transport and storage carbonic anhydrase, carboxy peptidase, Fe-S proteins and non – heme iron cytochromes of the electron transport chain – cytochrome P – 450 enzymes B_{12} nitrogen fixation and photosynthesis.

Anticancer activity of Pt complexes: Different types of active Pt - complexes, toxic effects of anticancer Pt - complexes, mechanism of anticancer activity, non – activity of trans – Platin.

References

1. James, E. Huheey, Ellen A. Keiter and Rechard L. Keitar Inorganic Chemistry. 4th Edition. Addison – Wesley (UNIT I, II, IV)
2. Shriver, Atkins and Longford Inorganic chemistry ELBS, 1994 (UNIT II)
3. Inorganic chemistry by J.D. Lee
4. Inorganic chemistry by Sathya Prakash
5. Inorganic chemistry by Cotton – Wilkinson
6. A.W. Adamson, Inorganic photochemistry (UNIT III)
7. Ajaykumar Bhagi, Inorganic and supra molecular chemistry.
8. Ivano,Bartini, Bioinorganic chemistry
9. Leninger, biochemistry
10. Asim K. Das, Bioinorganic chemistry,2008.

CORE COURSES VI – ORGANIC CHEMISTRY – II

Unit I **(18 hours)**

a. **Aliphatic nucleophilic substitution:** S_N1, S_N2 and S_NI mechanisms – effects of substrate structure, leaving group, attacking nucleophile and solvent – neighbouring group participation – substitution at allylic carbons and reactivity, ambident nucleophiles.

b. **Elimination reaction:** E1, E2, E1CB and Ei mechanisms – stereo chemistry of Elimimations Hoffman and Saytzeff rules – competition between elimination and substitution reactions – Chugaev reacation, dehydration of alcohols – dehydrohalogenation – Hoffman degradation – cope elimination – bredt's rule.

c. **Aliphatic electophilic substitution:** S_E1, S_E2 and S_EI mechanisms – effect of substrate structure, leaving group, attacking electrophiles and solvent – stork – enamine reaction – decarboxylation halogenation of aldehydes and ketones.

Unit II **(18 hours)**

a. **Aromatic compounds** : Elements of aromaticity – Huckel's and Craig's rule effects of aromaticity on bond length – ring current, non benzenoid aromatic compounds – aromatic character of three, five, seven and eight membered rings – anti – aromaticity systems with 2, 4, 6, 10, 14 and 18 electron systems, annulene and syndones – alternant and nonalternent hydrocarbons – chemicals consequences of aromaticity.

b. **Aromatic electrophilic substitution :** Aromatic ion mechanism – orientation and reactivity – nitration – halogenation, sulphonation, Friedal – Craft's reaction - Gattermann, Kolbe – Schmidt, Reimer – Teimen, Hauben – Housch reactions.

c. **Aromatic nucleophillic substitution :** Benzyne and intermediate mechanisms – effect of substrate structure, leaving groups, attacking nucleophiles and solvents. Selected reactions – Zeigler alkylation, Chichibabin reactions involving diazonium group as leaving group Cine substitution – Von- Richter reaction.

Unit III **(18 hours)**

a. Addition reactions : Addition to carbon - carbon multiple bond$LiAlH_4$ – $NaBH_4$ – tri tertiary butyl aluminium hydrides – mechanisticand stereochemical aspects of electrophylic addition nucleophilicfree radical addition, orientation and reactivity – Birch reduction –Diels alder reaction – Michael addition – Ozonolysis – carbenesand their addition to double bonds.

b. Addition to carbonyl group : Mannich, Crossed Cannizaro,Stobbe, Benzoin, formation of ketenes, Oppenauer oxidation, MPV reduction, Darzen's glycidic ester condensation, Wittigreaction.

Unit IV **(18 hours)**

a. **Molecular rearrangements :** Mechanism of the followingWagner Meerwin, dienone-phenol, Wolf, Lossen, Schmidt,Bayer Williger, Stevens, Wittig, Favorski rearrangements.

b. **Reagents in organic synthesis :** Complex metal hydride –$LiAlH_4$ – $NaBH_4$ – tri tertiary butoxy aluminium hydrides,Tri n-butyl tin hydride, Gilmann's reagents lithium dimethylCuprate, Lithium di isopropyl amide, dicyclohexyl carbo diimides 1-3

dithianes, tri methyl silyl iodide, DDQ, SeO_2,Phase transfer catalyst, Crown ethers, Merrifield resins.

Unit V **(18 hours)**

Natural products:

Terpenes : Structural elucidation and synthesis of alpha pinene, Camphor, and zingiberene.

Alkaloids: Structural elucidation and synthesis of quinine, reserpine,Morphine, and papavarine.

Vitamins : Physiological importance and structural elucidation ofVitamin B_6 and Vitamin-C.

References :

1. J.March "Advanced Organic Chemistry", Reaction mechanism and structure 4th edition Wiley,1999.
2. R.K. Bansal Organic Reaction Mechanism Tata Mcgraw Hill, 1975.
3. P.S. Kalsi, Organic Reaction and their Mechanisms, New Age International Publisher.
4. I.L.Finar, Organic Chemistry Vol II Vth Edition, ELBS – 1975.
5. O.P.Agarwal, Chemistry of Organic Natural Products, Vol I & II, Goel Publications.
6. T.H.Lowry and K.S.Richardson, Mechanism and Theorm in Organic Chemistry, Harper and Row, 1976.
7. Organic Reaction Mechanism by Gould.
8. Organic Reaction Mechanism by Liberlas.
9. Organic Reaction Mechanism by Chatwal.

CORE COURSE VII – INORGANIC CHEMISTRYPRACTICAL - II

I. Semi micro qualitative analysis of a mixture containing two common and two rare cations.
II. Colorimetric estimation of Copper, Iron and Nickel using photoelectric colorimeter.

Common cations

Lead, bismuth, copper, cadmium, antimony, Tin, Iron, Aluminium, Chromium, Manganese, Nickel, Cobalt, Zinc,Calcium, Barium, Strontium, Magnesium and Ammonium.

Less common cations

Tungsten,Thalium, Selenium,Tellurium, Molybdenum, Cerium,Zirconium, Beryllum and lithium.

CORE COURSE VIII – ORGANIC CHEMISTRY PRACTICAL II

I.Quantitative analysis of organic compounds

Estimation of Phenol, aniline, ketone, glucose, saponification value of an oil, iodine value of an oil.

II. Preparation of organic compounds : (Double stage)

1. Para – bromoaniline from acetanailide (bromination and hydrolysis)
2. Para – nitroaniline from acetanilide (Nitration and Hydrolysis)
3. Acetyl salicylic acid from methyl salicylate (hydrolysis and acetylation)
4. 1,3,5 – tribromo benzene from aniline (bromination and diazotisation)

MAJOR BASEDELECTIVE COURSE – II (A)
ANALYTICAL CHEMISTRY

Theory Hours : 5	**Course code : P20CH2EC2**
Exam Hours : 3	**Credits :5**
	Marks : Max marks -100
	Ext - 75
	Int - 25

OBJECTIVES

- To introduce concepts of various analytical techniques

UNIT - I **(15 hours)**

Instrumental Methods of Analysis: Principles and applications of extended X-ray absorption fine structure (EXAFS) – surface extended X-ray absorption (SEXAFS) – atomic absorption spectroscopy (AAS) – flame emission spectroscopy (FES) – turbidimetry – theory and applications.

UNIT -II **(15 hours)**

Data and Error Analysis: Various types of error – accuracy, precision, significant figures – frequency distributions, the binomial distribution, the Poisson distribution,n and normal distribution – describing data, population and sample, mean, variance, standard deviation,

Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t-Test, paired t-Test – analysis of variance (ANOVA) – correlation and regression.

Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – general polynomial equation fitting, linearizing transformations, exponential function fit – r and its abuse – multiple linear regression analysis, elementary aspects.

UNIT – III **(15 hours)**

Chromatography : Solvent extraction – principles of ion exchange, paper, thin-layer and column chromatography techniques – columns, adsorbents, methods, R_f values, McReynold's constants and their uses – HPTLC, HPLC techniques – adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques – methods, principles and uses.

UNIT – IV **(15 hours)**

Thermo Analytical Methods and Fluorescence Spectroscopy

Principles – instrumentations and applications of thermogravimetry analysis (TGA), Differential Thermal Analysis (DTA) and Differential Scanning Colorimetry (DSC) –thermometric titrations – types – advantages.

Basic aspects of synchronous fluorescence spectroscopy – spectral hole burning – flow cytometry – fluorometers (quantization) – instrumentation – applications.

UNIT- V **(15 hours)**

Electroanalytical Techniques: Electrochemical sensors, ion-sensitive electrodes, glass – membrane electrodes, solid-liquid membrane electrodes – ion-selective field effect transistors (ISFETs) – sensors for the analysis of gases in solution.

Polarography – principles and instrumentation – dropping mercury electrode – advantages – Ilkovic equation – applications of polarography – polarographic maxima – oscillographic polarography, AC polarography – cyclic voltammetry –advantages over polarographic techniques – chronopotentiometry – advantages – controlled potential coulometry.

Amperometric titrations: principles – techniques – applications – estimation of lead.

REFERENCES

1. D. B. Hibbert and J. J. Gooding, Data Analysis for Chemistry; Oxford University Press, UK, 2006.
2. J. Topping, Errors of Observation and Their Treatment; 4th Ed., Chapman Hall, London, 1984.
3. A. Braithwaite and J. F. Smith, Chromatographic Methods; 5th Ed., Springer, Germany; 1995.
4. V. K. Srivastava and K. K. Srivastava, Introduction to Chromatography; 2nd Ed., Holden Day, New York, 1985.
5. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, Instrumental Methods of Analysis; 6th Ed., CBS Publishers and Distributors, Chennai, 1986.
6. D. A. Skoog, D. M. West and D. J. Holler, Fundamentals of Analytical Chemistry, 7^{th} Ed., Harcourt College Publishers, Singapore, 2004.
7. A. Sharma, S. G. Schulman, Introduction to Fluorescence Spectroscopy; Wiley-Interscience, New York, 1999.
8. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy; 4^{th} Ed., Tata McGraw-Hill, New Delhi, 1994.
9. A. I. Vogel, Text Book of Quantitative Inorganic Analysis; 6th Ed., Longman, New Delhi, 2000.
10. D. C. Harris, Quantitative Chemical Analysis; 4th Ed., W. H. Freeman Publications,New York, 1995.
11. S. C. Gupta, Fundamentals of Statistics; 6th Ed., Himalaya Publications, Delhi,2006.

MAJOR BASED ELECTIVE COURSE –I(C)
SUPRAMOLECULAR CHEMISTRY

OBJECTIVES

1. To know the fundamentals of supramolecules.
2. To learn co-receptor molecules and multiple recognition
3. To study the supramolecular reactivity and catalysis.

UNIT I: Concepts of Supramolecular Chemistry

Concepts and languages of supramolecular chemistry – various types of non- covalent interactions – hydrogen bonds, C-H…X interactions, halogen bonds – π-π interactions, non–bonded interactions – various types of molecular recognition.

Crystal engineering of organic solids – hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs – concepts of different types of synthons based on non-covalent interactions – principles of crystal engineering and non-covalent synthesis – polymorphism and pseudopolymorphism – supramolecular isomorphism / polymorphism – crystal engineering of pharmaceutical phases.

UNIT II: Metallo Organic Frameworks

M.O.F (Metallo Organic Frameworks) – organometallic systems – combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. – design of nanoporous solids – interligand hydrogen bonds in metal complexes – implications for drug design – crystal engineering of NLO materials, OLED.

UNIT III: Co-receptor Molecules and Multiple Recognition

Dinuclear and polynulclear metal ion cryptates – linear recognition of molecular length by ditopic co-receptors – heterotopic co-receptors – cyclophane receptors, amphiphilic receptors and large molecular cages – multiple recognition in metalloreceptors – supramolecular dynamics.

UNIT IV: Supramolecular Reactivity and Catalysis

Catalysis by reactive macrocyclic cation receptor molecules – catalysis by reactive anion receptor molecules – catalysis with cyclophane type receptors – supramolecular metallocatalysis – cocatalysis – catalysis of synthetic reactions– biomolecular and abiotic catalysis.

Supramolecular chemistry in solution – cyclodextrin, micelles, dendrimers, gelators – classification and typical reactions – applications.

UNIT V: Supramolecular Devices

Supramolecular devices and sensors – various types of supramolecular devices – an overview – supramolecular photochemistry – molecular and supramolecular photonic devices – light conversion and energy transfer devices – molecular and supramolecular electronic devices – electronic conducting devices – molecular wires, modified and switchable molecular wires – molecular and supramolecular ionic devices – tubular mesophases, molecular protonics – switching devices – electro-photo switch – ion and molecule sensors – role of supramolecular chemistry in the development of nanoscience and technology.

REFERENCES

1. J. M. Lehn, Supramolecular Chemistry; VCH, Weinheim, Germany, 1995.
2. G. R. Desiraju, Crystal Engineering: The Design of Organic Solids; Elsevier, United States, 1989.
3. G. R. Desiraju, and T. Steiner, The Weak Hydrogen Bond in Structural Chemistry and Biology; Oxford University Press, Oxford, 1999.
4. G. A Jeffrey, Introduction to Hydrogen Bonding; Oxford University Press: UK, 1997.
5. J. M. Lehn, Transition Metals in Supramolecular Chemistry; John Wiley and Sons: New York, 1999.
6. G. R. Desiraju, Current Science; 2001, 81, 1038.
7. Web source:

(i) Crystal Growth and Design, http://www.pubs.acs.org/journals/cgdefu/index.html (ii) Crystal Engineering Communicationhttp://www.rsc.org/Publishing/Journals/ce/index.asp

SKILL ENHANCEMENT COURSE –I THEORY
TEXTILE CHEMISTRY (2Hours)

Theory Hours :2	**Course code : P20SET**
Exam Hours : 2	**Credits :2**
	Marks : Max marks -100
	Ext - 75
	Int - 25

OBJECTIVES

- This course aims at facilitating the students to understand the various techniques in textile industry and various processes in dying.

UNIT – I

Textile fiber and pretreatment: Classification of textile fibers – concept and techniques of Ginning, Sizing, Desizing, Scouring, Bleaching, and Mercerization- fiber identification tests (Flame test – microscopical & solubility test)

UNIT –II

Dye chemistry: Colour and sensation - theories of colour and chemical constitution – Witt's theory - chromospheres - auxochrome – chromogen - classification of dye based on application .

Unit-III

Technical terms in dyeing: M.L.ratio – % of shade– % of exhaustion – equilibrium absorption.

Non textile uses of dyes: Leather dyeing, paper dyeing, solvent dyes, food colours, hair colours and fluorescent brightening agents

Unit-IV

Dye bath assistants: Explanation and mechanism of exhausting agent, wetting agent, leveling agent, dispersing agent and carrier.

Fastness properties – Light, Washing Rubbings ,sublimation and perspiration fastness.

Unit-V

Textile proofing – Water proofs, moth proofing, mildew proofing & fire proofing.

Dyeing machineries: Padding mangle, Jigger, and Winch.

References:

1.Chemical Technology of fibrous Materials – F.sadov, M.Horchagin and A.Matetshy, MirPublishers.

2.The Identification of Textile Fibres – Bruno Nuntak.

3.Introduction to Textile Science -3rd edition, MaryoryL.Joseph.

4.Textile Chemistry –Vol.IIR.H.Peters, Elserier, Avesterdam.

5.Dyeing and chemical Technology of Textile fibres-5th Edition, E.R.Trotman,Charles Griffin &Co Ltd
6.Chemistry of dyes & Principles of Dyeing -V.A.Shenai, Sevak Publications.
7.Scouring and Bleaching E.R.Trotman, Charles Griffin & Co Ltd.
8.Text Book of Applied Chemistry- K.Kapur.
9.A Students Text Book of Textile Science- A.J.Hall.

EXTRA CREDIT COURSE

INTERNSHIP

SUBJECT CODE: INT Credit: 2 credits (Extra credits)

The curriculum includes the internship for students for 30 hours during the summer vacation after the second semester of all PG programs.

OBJECTIVES

The following are the intended objectives of internship training:

- To Enhance the employability skills of the students.
- To expose students to the industrial/Societal environment, which cannot be simulated in the classroom hence creating competent professionals for the industry and other organizations.
- To Provide possible opportunities to learn, understand, and sharpen the real-time technical/managerial skills required at the job.

Duration: 30 hours at the minimum

Period: During the summer vacation which could be completed within the third semester.

Assessment:

1. The assessment of the internship will be based on the feedback given by the internship provider and the report submitted by the student by the mentor.
2. After completion of the internship, the mentor has to make arrangements to get a proper training certificate from the industry/institution.
3. An abstract for details of the internship in the prescribed format has to be submitted by the departments to the COE on time.
4. Two credits are provided for the Internship as extra credits included under the Non-CGPA course for all PG programs.

LETTER FORMAT

GOVERNMENT COLLEGE FOR WOMEN (AUTONOMOUS), KUMBAKONAM

REQUEST LETTER FROM THE COLLEGE TO INTERNSHIP PROVIDER

To

……

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.....

Subject: REQUEST FOR INSTITUTIONAL/INDUSTRIAL TRAINING of M.A./M.Com/M.Sc Degree Programme,

Dear Sir/Madam,

You must be aware that our College has made internship mandatory for all M.A./M.Com/M.Sc students.

In view of the above, I request your good self to allow following students of our college for practical training in your esteemed organization. Kindly accord your permission and give at least 30 hours of training for the students to complete the internship.

S.NO	**NAME OF THE STUDENT**	**REG.NO**	**DISCIPLINE**

If vacancies exist, kindly plan for Campus/Off Campus Interviews for_____ batch passing out students in above branches.

A line of confirmation will be highly appreciated.

With warm regards,

Yours sincerely,

Head of the Department.

GOVERNMENT COLLEGE FOR WOMEN (AUTONOMOUS), KUMBAKONAM

REQUEST LETTER FROM THE COLLEGE TO INTERNSHIP PROVIDER

To

……

.....

.....

Subject: REQUEST FOR INSTITUTIONAL/INDUSTRIAL TRAINING of M.A./M.Com/M.Sc Degree Programme,

Dear Sir/Madam,

Our Students have undergone internship training in your esteemed Organization in the previous years. I acknowledge the help and the support extended to our students during training in previous years.

In view of the above, I request your good self to allow our following students for practical training in your esteemed organization. Kindly accord your permission and give at least 30 hours of training for the students to complete internship.

S.NO	NAME OF THE STUDENT	REG.NO	DISCIPLINE

If vacancies exist, kindly do plan for Campus/Off Campus Interview for_____ batch passing out students in above branches.

A line of confirmation will be highly appreciated.

With warm regards,

Yours sincerely,

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Head of the Department.

FORM - 1

INTERNSHIP DETAILS (THIS WILL BE PREPARED IN CONSULTATION WITH FACULTY MENTOR AND TO BE MAINTAINED BY tHe department)

Student

Name:_____Reg.No._____Class_____

Campus Address: _____

_____

Phone:_____Email: _____

Internship Provider

Name:_____

Title:_____

Company/Organization:_____

Internship Company Adress_____

_____

_____

Phone:_____Email:_____

Faculty Mentor

Name:_____Phone: _____

Designation:_____Department:_____

Academic Credit Information

Internship Title: _____

Date of Initiation:_____Date of Completion: _____

Total Hours: _____

FORM - 2

STUDENT'S DAYWISE LOG ENTRY

Name and Reg.No. of the Student: Name and address of the Internship Provider:

Period of Internship: From:		**To:**		
Date	**Hours**	**Details of work done**	**Signature of the Student**	**Signature of the Supervisor**

Signature of the Mentor: Signature of the Internship Provider:

FORM -3

SUPERVISOR EVALUATION OF CANDIDATE

Student Name: _____ Date:_____

Work Supervisor:_____Title:_____

Company/Organization:_____

Internship Address:_____

Dates of Internship: From _____To_____

Please evaluate your candidate by indicating the frequency with which you observed the following behaviors:

Parameters	**Needs improvement**	**Satisfactory**	**Good**	**Excellent**
Interest in work				
Punctuality				
Reliability				
Responsibility				
Communication				
Team work				
Overall performance				

Additional comments, if any:

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Signature of Internship Provider

FORM - 4

STUDENT FEEDBACK OF INTERNSHIP (TO BE FILLED BY STUDENTS AFTER INTERNSHIP COMPLETION)

Student Name:_____ Class: _____

Internship Provider: _____

Address: _____

Title of Internship :_____

Supervisor Email:_____

Faculty Mentor:_ _____

Indicate the degree to which you agree or disagree with the following statements.

This experience has	**Strongly Agree**	**Agree**	**Disagree**
Given me the opportunity to explore a career field			
Allowed me to apply classroom theory to Practice			
Expanded my knowledge			
Helped me develop my written and oral communication skills			
Given me a chance to improve my interpersonal skills			
Provided me with contacts which may lead to future employment			
Helped me clarify my career goals			

Considering your overall experience, how would you rate this internship?

(Tick one).(Satisfactory/ Good/ Excellent)

Signature of the Student

FORM – 5

EVALUATION SHEET (FOR MENTOR)

S.NO	NAME OF THE STUDENT	REG.NO	NO. OF ACTUAL INTERNSHIP HOURS	GRADE*

* Evaluation based on report submitted by the student and evaluation by Internship provider. (Excellent/ Very good/ Good)

Signature of the Head of the Department

Signature of the Mentor

SEMESTER III
CORE COURSE IX – INORGANIC CHEMISTRY – III

Unit I **(18 hours)**

Electronic Spectroscopy: Electronic configuration, Terms, States and Microstates, Derivation of term symbols(p^2, d^2) and arranging the various terms according to their energies. Spectroscopic terms – Effect of inter electronic repulsion and spin – orbit coupling – Racah parameters B and C, R-S coupling and jj coupling. Selection rules and the breakdown of selection rules – Group theoretical explanation. Ground states of free ions for d^n systems – Oh and Td systems and the corresponding energy level diagrams – mixing of orbits. Orgel diagram – characteristics – prediction and assignment of transitions for d^n weak field cases. Tenabe – Sugano diagrams – characteristics – prediction and assignment of transition for weak field and strong field. Calculation of B and 10dq for simple Octahedral complexes of Co and Ni – Change transfer spectra.

Unit II **(18 hours)**

IR and Raman spectroscopy:

Combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like H_2O, ClF_3, NO_3, ClO_3. Effect of Co-ordination on ligand vibrations – uses of group vibrations in the structural elucidation metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethylsulphoxide. Effect of isotopic substitution on the vibtational spectra of molecules – Vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of CO stretching vibrations (Group theoretical treatment).

Mossbauer Spectroscopy:

Mossbauer transition and Doppler effect – Isomer shift quardrupole effect of magnetic field on spectra – simple applications to iron and tin compounds.

Unit III **(18 hours)**

NMR Spectroscopy:

Chemicals shift and coupling (spin – spin coupling involving different nuclei H^1, P^{31}, C^{13}) interpretation and applications to Inorganic compounds. Effects of quadrupolar nuclei on the H^1 NMR Spectrum. NMR paramagnetic molecules – isotopic shifts, contact and pseudocontact interactions – Lanthanide shift reagents. Applications of P^{31}, C^{13}, H^1NMR of inorganic molecules.

Unit IV **(18 hours)**

EPR Spectroscopy:

Basic principles – characteristics of g – Hyperfine splitting on various structures – Bis (salicylaldimine copper(II) – factors affecting the magnitude of the g values of transition metal ions – Three conditions (i) Spin – Orbit coupling crystal field (ii) Strength of the crystal breaking the spin – orbit coupling (iii) very large crystal field Ni(II) octahedral complex – Cu^{2+} in a tetrahedral complex - Cu^{2+} in a tetragonal field – Zero field splitting – Line widths in solid state EPR Spin lattice – Spin relaxation – exchange processes.

Magnetic properties:

Types of magnetism – Dia – Para – ferro and antiferro magnetism. Magnetic properties of free ions – Temperature independent paramagnetism. Anamalous magnetic moment – ferromagnetic and antiferromagnetic exchanges.

Unit V **(18 hours)**

X – Ray Crystallography:

Solid state : Difference between point group – screw axis – glide plane Crystal symmetry elements – crystal classes – crystal systems – unit cell – bravis lattices – asymmetric unit space group – equivalent positions – relationship between molecular symmetry and crystallographic symmetry – basic concepts, the concept of reciprocal lattice and its application – X – ray diffraction by single crystal – structure factor – systematic absences – determination of space group – heavy atom method.

Neutron diffraction – elementary treatment – comparison with X – ray diffraction Electron diffraction – basic principles.

References:

1. B.N.Figgis, Introduction to Ligand Fields, Willey Eastern, New Delhi, (Unit I,II,III & IV)
2. James E Huheey, Ellen A.Keither and Richard L.Keiter, In organic Chemistry, 4^{th} edition.
3. R.S.Drago, Physical Methods in Inorganic Chemistry.
4. A.F.A.Kettle, Co-ordination Compounds, ELBS (Unit I,II,III & IV).
5. D.F.Shriver, P.W.Atkins and C.H.Langford, Inorganic Chemistry, 2^{nd} Editions.
6. Silverstein, Advanced Spectroscopy.

7. William Kemp, Spectroscopy.
8. Y.R.Sharma,Spectroscopy.
9. Jagmohan, Spectroscopy.

CORE COURSE X – ORGANIC CHEMISTRY – III

Unit I **(18 hours)**

Organic photochemistry: Fundamental concept – Jablonski diagrams – energy transfer characteristics of photo reduction and photo oxidation – photoreaction of ketones and enols norrish type I and II – reactions – photo – chemistry of alkenes, dienes and aromatic compounds – photo sensitation photo additions – Barton reaction – Paterno Buchi reaction.

Pericyclic reactions: Concerted reactions – Stereochemistry – orbital symmetry and correlation diagram – Frontier molecular orbital approach – Woodward – Hoffmann rules – electrocyclicreactions – cycloaddition

Reactions – selection rules – sigmatropic rearrangements – selection rules with simple molecules – 1,and 1,5 hydrogen shifts – Cope and Claisen rearrangements.

Unit II **(18 hours)**

Ultra violet and visible spectroscopy: Basis principle of electronic transitions – correlation of energy change with electronic transitions – instrumentation and sample handling techniques – Application of UV- Visible spectroscopy – Woodward – Fieser – Scott rules – application to conjugated dienes, trienes and poleynes – unsaturated carbonyl compounds – conjugated cyclic ketones – acetophenones – benzene and its substituted derivatives.

Infrared spectroscopy: Instrumentation and sampling techniques – types of stretching and bending vibrations – characteristic group frequencies –(internal and external)-quatitative studies – organic structure determinations, finger printregion – identification of functional groups – hydrogen bonding(intermolecular and intra molecular).

Unit III **(18 hours)**

NMR Spectroscopy:

Chemical and magnetic non-equivalence, chemical shift – coupling constant – first and second order proton spin – spin splitting dependence of J on dihedral angles – vicinal and geminal coupling constants – karplus equation – long range coupling constants – influences of stereo chemical factors on chemical shift of protons simplification of complex spectra – double resonance techniques – shift reagents – chemical spin decoupling of rapidly exchangeable protons – OH, COOH, SH, NH,

NH_2 – an elementary treatment of NOE phenomenon – to techniques – COSY – NOSEY.

C^{13} NMR Spectroscopy : Basic principles **–** FT NMR Relaxation – broad band decoupling – off resonance decoupling – calculation of chemical shifts for simple aliphatic and aromatic compounds – conformation and chemical shift correlation – peak assignments – importance of NOE phenomenon in C^{13} spectroscopy.

Unit IV **(18 hours)**

Mass Spectrometry: Basic principles – resolutions – EI and CI methods – base peak – recognition of molecular ion peak – FAB fragmentation – general rules – nitrogen rule – McLafferty rearrangement – ortho effects – importance of metastable peaks.

Electron spin resonance spectroscopy: Basic principles – comparison between esr and nmr spectra hyperfine splitting – factors affecting the magnitude of values applications to organic free radicals, Methyl and naphthyl radicals.

Optical rotatory dispersion and circular dichroism: Cotton effect – ORD curves – axial haloketone rule and its applications – octant rule – its applications – applications of ORD to determine absolute configuration of monocyclic ketones.

Unit V **(18 hours)**

Steroids: Classification – structural elucidation of cholesterol – (synthesis not required) – structural elucidation of vitamin D – estrone – progesterone, ergosterol, androsterone and cortisone – classification and functions of prostoglandins

Heterocyclics: Synthesis and reaction of azoles – pyrazole, imidazole, oxazole and thiazole.

Refernces

1. C.N. Banwell, Fumdamentals of molecular Spectroscopy.
2. P.M.Silverstein, F.X.Wester, Spectroscopic Identification of Organic compounds.
3. P.S.Kalsi, Spectroscopic of Organic compounds.
4. W.Kemp, Organic Spectroscopy.
5. Y.R. Sharma Elementary Organic Spectroscopy.
6. J.D. Coyle, Organic Photochemistry, 1985.
7. G. R.Chatwall Organic Photochemistry,1998.
8. G,M. Barrow, Introduction to molecular Spectroscopy, 1964.
9. Jagmohan, Organic Spectroscopy.

CORE COURSE XI – PHYSICAL CHEMISTRY – II

UNIT I **(18 hours)**

Group Theory

Elements of Group Theory – properties of group and subgroup – classes – group multiplication tables – isomorphism, group - symmetry elements and symmetry operations – interrelations among symmetry operations – generators – point groups of molecules – Matrix representation theory – Consequences of great orthogonality theorem and construction of character tables – characters reducible and irreducible representation – Direct products and correlation tables.

Application of group theory to IR, Raman and electronic spectra – Projection operators – SALC procedure – evaluation of energies and MO's for system like ethylene – butadiene planar monocyclic aromatic Compounds – hybridisation schemes of orbitals.

Unit – II **(18 hours)**

Quantum Chemistry – II

Application of SWE to simple harmonic oscillator (Hermite Polynomial, eigen function, eigen values – rigid rotator with free Axis (SWE) in polar coordinates, separation of angular functions and their solution, Legendre and associated Legendre polynomials, degencracy of rotational states – hydrogen and hydrogenlike atoms (separation of angular and radial functions and solution to radial equation, Laguerre and associated Laguerre polynomials, quantum numbers, space quantization, electron spin) – the antisymmetry or Pauli exclusion principle and siater determinant – ground state helium atom).

Unit III **(18 hours)**

Molecular Spectroscopy

Infra red spectroscopy: Vibrational spectra selection rule – (fundamentals absorption, first and second overtones, hot bands etc.) vibrational spectra of diatomic molecules, selection rule for the rigid rotor – harmonic oscillator mode – relative intensities – coupling and rotation of vibration – linear molecules and symmetric top molecules(parallel and perpendicular bands).

Raman spectroscopy: Raman effect elastic and inelastic scattering – selection rule – pure rotational raman spectra (linear, spherical top, symmetric top and asymmetric top molecules – vibrational raman spectra – polarization of light and

Raman effect – comparison of IR and Raman spectra – simplemolecule – mutual exclusion principle – Fermi resonance – laser Raman spectroscopy – elementary treatment only.

Unit IV **(18 hours)**

Statistical Thermodynamics

Calculation of thermodynamic probability of a system – Difference between thermodynamic and statistical probability – Ensembles, phase space – ergodic hypothesis – definition of micro and macro states – different methods of counting macro states – distinguishable and indistinguishable particles – classical statistics – derivation of Maxwell – Boltzmann distribution law.

Partition Function

Translational, rotational, vibrational, Electronic – calculation of enthalphy, internal energy, Entropy and other thermodynamic functions – application of partition functions to mono atomic and diatomic molecules.

Unit V **18 hours)**

Surface phenomena: Adsorption and free energy reaction relation at inter – phase – physisorption and chemisorption – potential energy diagram – Lennard- Jones plot – Langmuir, BET isotherm – surface area determination – heats of adsorption, determination – adsorption from solution – Gibbs adsorption isotherm.

Role of surfaces in catalysis: Semiconductor catalysis – n and p type surfaces – kinetics of surface reactions involving adsorbed species – Langmuir – Hinshelwood, mechanism of bimolecular reaction – Langmuir – Rideal mechanism of bimolecular reaction – Rideal – Eler mechanism.

References:

1. F.A.Cottan, Chemical Application of Group Theory 2nd edition, Wiley – Baster(1971)
2. R.L.Flowry,Jr,Symmetry Groups – Prentice Hall, NewJersy(1980)
3. C.N.Banwell, Fundamentals of Molecular Spectroscopy, Tata Megraw Hill edition(1993)
4. R.K.Prasad, Quantum Chemistry, 2nd edition.
5. Gupta, Statistical Thermodynamics.
6. G.C.Bond, Heterogeneous Catalysis – Principles.
7. Mathematics for quantum chemistry, J.M.Anderson, Benjamin.
8. Introductory quantum chemistry, A.K.Chandra, Tata – MeGraw Hill edition.
9. Molecular quantum mechanics, P.W.Atkins, Clarenden.

10. Levine, Quantum Chemistry.
11.K.V.Raman, Group theory and its applications.

CORE COURSE XII – PHYSICAL CHEMISTRY PRACTICAL – I

1. Determination of molecular weight of substance by Transition Temperature method.
2. Determination of molecular weight of substance by Rast's method.
3. Determination of Critical Solution Temperature(CST) of phenol – water system and effect of impurity on CST.
4. Study of phase diagram of two components forming a simple eutectic.
5. Study of phase diagram of two components forming a compound.
6. Kinetics – Acid hydrolysis of an Ester – Comparison of strength of acids.
7. Kinetics – Acid hydrolysis of an Ester – Determination of Energy of Activation(Ea)
8. Kinetics – Persulphate – Iodine reaction – Determination of order, effective of ionic strength on rate constant.
9. Adsorption – Oxalic acid/Acetic acid on charcoal using Freundlich isotherm.

References:

1. Findlay's Practical Physical Chemistry Revised and edited by B.P.Levitt, 9th edition.
2. J.N.Gurtur and R.Kapoor, Advanced Experimental chemistry, Voli,Chand &co., Ltd, New Delhi.

ELECTIVE COURCE – III MEDICINAL CHEMISTRY

Unit I

Introduction – definition of allergy, intolerance and side, effects, drug induced side effects – tolerance, resistance and dependence.

First aid for accidents – rules of first aid – cuts, abrasions, bruises,bleeding, fractures, burns, fainting and poisonous bites – detection of hallucinogens and poisons – antidotes for poisoning.

Unit II

Analgesics : Classification – non narcotic and narcotic analgesics – antipyretic analgesics – paracetamol, phenacetin – synthesis and uses, Asprirn –synthesis, uses and toxic effects. Anti inflammatory analgesics – ibuprofen and indo methacin – synthesis,uses and toxic effects.

Unit III

Antibiotics : Introduction – classification pencillins, streptomycin and chloromphenicol – synthesis, toxic effects and uses. Antifungal antibiotics – hystatin.

Anti malarials: Quinine synthesis,uses and toxic effects.

Unit IV

Vitamins : Classification –source and deficiency. Vitamin A,D,E,K,B complexes(B_1, B_2 , B_6, and B_{12},), folic acid and vitamin – C.

Hormones: Definition – classification – thyroxin, oxytocin, insulin, progesterone and andestrone and its importance and uses

Unit V

Ageneral study of the following classes of compounds

1. Sedatives, hypnotics and transquilizers.
2. Antiseptics and disinfectants.
3. Anti cancer drugs.
4. Diabetic & hypoglycemic drugs.

Reference :

1. Alfred Burger, “Medicinal Chemistry” part I & II, 3rd edn, Willey interscience.
2. Goodman and Gilman “Pharmacology and Pharmacothearputics” .
3. Ahsulosh Kar, “Medicinal chemistry” Wiley Eastern, Madras.

4. Harkrishan singh and V.K.Kapoor, "Organic pharmaceutical Chemistry", Vallabh Prakashan, Delhi.
5. I.L.Finar, "Organic Chemistry" Vol I & II ELBS.
6. Jayashree ghosh, a text book of "Pharmaceutical Chemistry".

MAJOR BASED ELECTIVE COURSE - II
II (C) BIO-ORGANIC CHEMISTRY

Theory Hours :6	**Course code : P20CHC309**
Exam Hours : 3	**Credits :5**
	Marks : Max marks -100
	Ext - 75
	Int - 25

OBJECTIVES

1. To learn the preparation, properties of amino acids and proteins.
2. To study the activity of enzymes and cofactors.
3. To know basics of lipids and nucleic acids.
4. To learn the concept of bioenergetics.
5. To learn the principles of lead and analogue synthesis.

UNIT I: Amino Acids and Proteins

Structure, classification, synthesis and properties of amino acids – biosynthesis of amino acids – peptides – N-terminal and C-terminal residue analysis – solid phase peptide synthesis.

Proteins – classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins – biological roles of proteins.

UNIT II: Enzymes and Cofactors

Chemical nature of enzymes – characteristics of enzymes – colloidal nature, catalytic nature.

Mechanism of enzymes – Michaelis-Menten hypothesis – Fischer's lock and key model – regulation of enzyme activity.

Stucture and biological functions of coenzyme A, NAD+, FAD and vitamin B12.

UNIT III: Lipids and Nucleic Acids

Lipids – definition – simple lipids – fats and oils – compound lipids – phospholipids, glycolipids – physical properties – solubility, melting point, surface tension, emulsification and geometric isomerism – chemical properties – reaction involving -COOH group, -OH group and double bonds. Nucleic Acid – definition – nucleosides and nucleotides – deoxyribonucleic acid (DNA) – internucleotides linkages – base composition – double helical structure.

UNIT IV: Bioenergetics

Concept of energy – thermodynamic principles – first law, second law, combining the two laws – relationship between standard free energy change and equilibrium constant. Standard free energy values of chemical reactions – Adenosine triphosphate (ATP) as universal currency of free energy in biological systems – ATP hydrolysis and equilibria of coupled reactions – inter conversion of adenine nucleotides.

UNIT V: Lead and Analogue Synthesis

Designing organic synthesis – disconnection approach – synthons and synthetic equivalents – one group disconnections: alcohol, acid and ketone – functional group interconversions. Asymmetric synthesis – basic principles – stereoselective and stereospecific reactions – reagents, catalysts and their applications (wherever applicable) in alkylation and hydrogenation – Jacobsen's catalyst – Evan's catalyst.

REFERENCES

1. J. L. Jain, Fundamentals of Biochemistry; S. Chand and Co., New Delhi, 2007 [Unit- I, II, III, IV].
2. N. C. Price and L. Stevens, Fundamental of Enzymology; Oxford University Press, UK, 1999 [Unit-II].
3. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry: Part-A and Part-B; 5th Ed., Springer, Germany, 2008 [Unit-I, II, III].
4. S. Warren, Designing Organic Synthesis: The Disconnection Approach; 2nd Ed., Wiley, New York, 2008 [Unit-V].
5. H. B. Kagan, Asymmetric Synthesis; Thieme Medical Publishers, Germany, 2009 [Unit – V].

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MAJOR BASED ELECTIVE COURSE – I (B)

CHEMISTRY OF NANOSCIENCE

Theory Hours : 5 **Exam Hours : 3**	**Course code : P20CH1EC1** **Credits :4** **Marks : Max marks -100** **Ext - 75** **Int - 25**

OBJECTIVES:

- To impart the knowledge of Nano chemistry.
- To know about Nano materials and how it is differs from bulk materials.

UNIT I

Synthetic Methods: Definition of nano dimensional materials – historical milestones – unique properties due to nanosize, quantum dots, classification of nano materials. General methods of synthesis of nanomaterials – hydrothermal synthesis, solvothermal synthesis – microwave irradiation– sol-gel and precipitation technologies– combustion flame – chemical vapour condensation process – gas-phase condensation synthesis – reverse micelle synthesis – polymer-mediated synthesis –protein microtubule-mediated synthesis – synthesis of nano materials using microorganisms and other biological agents – sono chemical synthesis – hydrodynamic avitation. Inorganic nano materials – typical examples – nanoTiO_2 /ZnO/CdO/CdS, organic nanomaterials – examples – rotaxanes and catenanes

UNIT II

Characterisation of Nanoscale Materials: Principles of Atomic Force Microscopy (AFM) – Transmission Electron Microscopy (TEM) Resolution and Scanning Transmission Electron Microscopy (STEM) – Scanning Tunneling Microscopy (STM) – Scanning Near field Optical Microscopy (SNOM).Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.

UNIT III

Reactions in Nanoparticles: Reactions in nano space – nano confinement – nanocapsules Cavitands, cucurbiturils, zeolites, M.O.Fs, porous silicon, nano catalysis.

Applications of nano materials : Ferro electro material, coating, molecular electronics and nano electronics, biological and environmental membrane based application, polymer application.

UNIT IV

Carbon Clusters and Nanostructures: Nature of carbon bond − new carbon structures − carbon clusters – discovery of C60−alkali doped C60−superconductivity in C60−larger and smaller fullerenes. Carbon nano tubes – synthesis − single walled carbon nano tubes − structure and characterization − mechanism of formation − chemically modified carbon nano tubes −doping − functionalizing nano tubes – applications of carbon nano tubes. Nano wires −synthetic strategies − gas phase and solution phase growth – growth control− properties.

UNIT V

Nanotechnology and Nanodevices: DNA as a nano material – DNA – knots and junctions, DNA – nano mechanical device designed by Seeman. Force measurements in simple protein molecules and polymerase – DNA complexes–molecular recognition and DNA based sensor. Protein nanoarray, nano pipettes, molecular diodes, self-assembled nano transistors, nanoparticle mediated transfection.

REFERENCES

1. C. N. R. Rao, A. Muller and A. K. Cheetham (Eds), The Chemistry of Nanomaterials: Vol. 1 and 2; Wiley-VCH;Germany, Weinheim, 2004.
2. C. P. Poole, Jr: and F. J. Owens, Introduction to Nanotechnology; Wiley Interscience, New Jersey, 2003.
3. K. J. Klabunde (Ed), Nanoscale Materials in Chemistry; 2nd Ed., Wiley- Interscience, New York, 2009.
4. T. Pradeep, Nano: The Essentials in Understanding Nanoscience and Nanotechnology; 1st Ed., Tata McGraw Hill, New York, 2007.
5. H. Fujita (Ed.), Micro machines as Tools in Nanotechnology; Springer-Verlag, Berlin, 2003.
6. BengtNolting, Methods in Modern Biophysics; 3rd Ed., Springer-Verlarg, Berlin, 2009.
7. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties, Elsevier, Chennai, 2000.
8. W. Kain and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life; 2nd Ed., John-Wiley R Sons, New York, 2013.
9. T. Tang and P. Sheng (Eds), Nanoscience and Technology, Novel Structures and Phenomena; Taylor andFrancis, New York, 2003.

10. A. Nabok, Organic and Inorganic Nanostructures; Artech House, Boston, 2005.
11. E. A. Rietman, Molecular Engineering of Nanosystems; Springer-Verlag, New York, 2001.
12. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/
13. Nanoletters - http://pubs.acs.org/journals/nalefd/index.html
14. Nanotation - http://www.acsnanotation.org/

CORE COURSE XIII – PHYSICAL CHEMISTRY – III

Unit- I **(18 hours)**

Group Theory

Elements of Group Theory – properties of group and subgroup – classes – group multiplication tables – isomorphism, group - symmetry elements and symmetry operations – interrelations among symmetry operations – generators – point groups of molecules – Matrix representation theory – Consequences of great orthogonality theorem and construction of character tables – characters reducible and irreducible representation – Direct products and correlation tables.

Application of group theory to IR, Raman and electronic spectra – Projection operators – SALC procedure – evaluation of energies and MO's for system like ethylene – butadiene planar monocyclic aromatic Compounds – hybridisation schemes of orbitals.

Unit – II **(18 hours)**

Quantum Chemistry – II

Application of SWE to simple harmonic oscillator (Hermite Polynomial, eigen function, eigen values – rigid rotator with free Axis (SWE) in polar coordinates, separation of angular functions and their solution, Legendre and associated Legendre polynomials, degeneracy of rotational states – hydrogen and hydrogenlike atoms (separation of angular and radial functions and solution to radial equation, Laguerre and associated Laguerre polynomials, quantum numbers, space quantization, electron spin) – the antisymmetry or Pauli exclusion principle and slater determinant – ground state helium atom)

Unit III **(18 hours)**

Molecular Spectroscopy

Infrared spectroscopy: Vibrational spectra selection rule – (fundamentals absorption, first and second overtones, hot bands etc.) vibrational spectra of diatomic molecules, selection rule for the rigid rotor – harmonic oscillator mode – relative intensities – coupling and rotation of vibration – linear molecules and symmetric top molecules(parallel and perpendicular bands).

Raman spectroscopy: Raman effect, elastic and inelastic scattering – selection rule – pure rotational raman spectra (linear, spherical top, symmetric top and asymmetric top molecules – vibrational raman spectra – polarization of light and

Raman effect – comparison of IR and Raman spectra – simple molecule – mutual exclusion principle – Fermi resonance – laser Raman spectroscopy – elementary treatment only.

Unit IV **(18 hours)**

Statistical Thermodynamics

Calculation of thermodynamic probability of a system – Difference between thermodynamic and statistical probability – Ensembles, phase space – ergodic hypothesis – definition of micro and macro states – different methods of counting macro states – distinguishable and indistinguishable particles – classical statistics – derivation of Maxwell – Boltzmann distribution law.

Partition Function

Translational, rotational, vibrational, Electronic – calculation of enthalphy, internal energy, Entropy and other thermodynamic functions – application of partition functions to mono atomic and diatomic molecules.

Unit V **(18 hours)**

Surface phenomena: Adsorption and free energy reaction relation at inter – phase – physisorption and chemisorption – potential energy diagram – Lennard- Jones plot – Langmuir, BET isotherm – surface area determination – heats of adsorption, determination – adsorption from solution – Gibbs adsorption isotherm.

Role of surfaces in catalysis: Semiconductor catalysis – n and p type surfaces – kinetics of surface reactions involving adsorbed species – Langmuir – Hinshelwood, mechanism of bimolecular reaction – Langmuir – Rideal mechanism of bimolecular reaction – Rideal – Eler mechanism.

References:

F.A.Cottan, Chemical Application of Group Theory 2nd edition, Wiley – Baster(1971)

R.L.Flowry,Jr,Symmetry Groups – Prentice Hall, NewJersy(1980)

C.N.Banwell, Fundamentals of Molecular Spectroscopy, Tata Megraw Hill edition(1993)

R.K.Prasad, Quantum Chemistry, 2nd edition.

Gupta, Statistical Thermodynamics.

G.C.Bond, Heterogeneous Catalysis – Principles.

Mathematics for quantum chemistry, J.M.Anderson, Benjamin.

Introductory quantum chemistry, A.K.Chandra, Tata – MeGraw Hill edition.

Molecular quantum mechanics, P.W.Atkins, Clarenden.

Levine, Quantum Chemistry.

K.V.Raman, Group theory and its applications.

CORE COURSE XII- RECENT TRENDS IN CHEMISTRY

UNIT –I **(18 hours)**

Introduction to computing and networking:

Introduction to computers and computing - hardware – basic organization of a computer CPU –main memory- secondary- i/odevices – software system and applications of software-high and low level languages compilers- algorithms and flow charts.

Introduction to networking –computer networks- LAN,WAN, intranet and internet –worldwide web- internet for chemists-online search of chemistry data bases-e-journals- search engines for chemistry**.**

Unit-II **(18 hours)**

Nano chemistry

Introduction to nanotechnology- molecular nanotechnology- nanomanipulator, nanotweezers, atom manipulation – nanomaterials-preparation of nanomaterial-plasma arcingmethod, chemical vapor deposition method,electrodeposition method-applications of nanometrials(batteries, medical implants,motor vehicles and aircraft- nanotubes-properties and uses of nanotubesnanomedicines,environmental applications.Fullerenes-properties &uses.

(18 hours)

Unit-III

Research methodology

Introduction to primary sources (journals name and patent),secondary sources (chemical abstract,Dictionary,Monographs and Review articles), Chemical abstracts- Subject index –author index and formula index and other indexes with examples-current contents – organization -methods of using the titles and index-preparation and presentation of research papers in journals and seminars.

Unit –IV **(18 hours)**

Green chemistry:

Priniciples(12)- inception-scope areas-green solvents-biocatalyst and biocatalysis – synthesis of safer product.

Green chemistry-photochemical principles- photooxidation- photodegradation-removal of hazardous chemicals from water-cleaner production concept - implementation- Government role.

Unit-V **(18 hours)**

Molecular modeling basics

Molecular modeling- coordinate systems – cartesian and internal coordinate systems-bond lengths, bond angles and torsion angles, potential energy surfaces. Molecular mechanics-application and parameterization-advantages and limitations of force fields.

References:

1.E.Balaguruswamy, Programming in ANSIC",Tata McGraw Hill,2nd edition,New Delhi,1999.

2.Robert Lafore,"Object Oriented Programming in Turbo C++", Galgotia, New Delhi,1995.

3.K.V.Raman ,Computers in chemistry, Tata McGraw Hill, New Delhi1993.

4.M.M.Srivatsava,Rashmi saneni chemicals for green environment, Narosa publishing house, New Delhi.

5. T.Pradeep " Nano the essentials- understanding nano science and nano technology" Tata McGraw Hill publishing Ltd, New Delhi.

7. A.R.Leach, Molecular Modeling Principles and applications, 2nd edition prentice Hall,2001.

8. Green chemistry, Ahluwalia.

ELECTIVE COURSE - IV(B)

INDUSTRIAL CHEMISTRY

UNIT I (15 hours)

Basic Ideas and Industrial Wastes: Basic idea about unit operation – flow chart – chemical conversion – batchversus continuous processing – chemical process selection – design – chemicalprocess control.

Types of industrial wastes – treatment of wastes or effluent with organicimpurities – treatment of wastes or effluent with inorganic impurities –treatment of some important chemical wastes.

UNIT II (15 hours)

Petroleum and Petrochemicals: Introduction – saturated hydrocarbons from natural gas – uses of saturatedhydrocarbons – unsaturated hydrocarbons – acetylene, ethylene, propylene,butylene – aromatic hydrocarbons – toluene and xylene.Preparation of rectified spirit from beat – methylated spirit – preparation ofabsolute alcohol from rectified spirit – petrochemicals in India.

UNIT III (15 hours)

Manufacture of Cement: Introduction – types of cement – high alumina cement, water proof cement, slagcement, acid resisting cement, white cement, coloured cement, Pozzolanacement.Setting of cement – properties of cement – testing of cement – uses of cement –concrete – cement industries in India.

UNIT IV (15 hours)

Pulp and Paper and Manufacture of Paper: Introduction – manufacture of pulp – types of pulp – sulphate or craft pulp,soda pulp, Rag pulp – beating, refining, filling, sizing and colouring.Calendaring – uses – paper industries in India.

UNIT V (15 hours)

Soaps, Detergents and Perfumes: Introduction – types of soaps – hard and soft soaps – manufacture of soap (hotand continuous process only) – cleansing action of soap – detergents – surfaceactive agents – biodegradability of surfactants, amphoteric detergents.Introduction – production of natural perfumes – flower perfumes – jasmine,rose and lily – production of synthetic perfumes – muscone and nitro-musks.

REFERENCES

1. B. K. Sharma, Industrial Chemistry; 8th Ed., Goel Publishing House, New Delhi, 1997. (Unit–I, II, III, IV and V)

2. R. N. Shreve, and J. A. Brink Jr. Chemical Process Industries; 4th Ed., McGraw Hill, Toronto, 1977. (Unit–I, II, III, IV and V)

3. A. C. S. Brain, Production and Properties of Industrial Chemicals; Reinhold, New York, 1989. (Unit–I)

SEMESTER - IV
ELECTIVE COURSE - IV (B)
EXPERIMENTAL METHODS IN CHEMISTRY

Theory Hours :6	**Course code : P20CHC4EC4**
Exam Hours : 3	**Credits :4**
	Marks : Max marks -100
	Ext - 75
	Int- 25

OBJECTIVES

- To learn about the basic concepts of surface imaging and application.
- To learn about chemical analysis, electro analytical techniques, separation methods and applications.

UNIT I

SURFACE IMAGING: Basic concepts in surface imaging – Principle, Instrumentation and Applications –secondary electron microscopy(SEM), secondary Auger microscopy(SAM), scanning probe microscopy(SPM), scanning tunneling microscopy(STM), transmission electron microscopy(TEM).

UNIT II

CHEMICAL ANALYSIS: Non-destructive techniques – X-ray absorption , Diffraction and fluorescence spectroscopy – theory, instrumentation and applications. Destructive technique – Atomic absorption spectroscopy – principle, instrumentation–EMR sources – cells – furnaces – detectors – interferences and their corrections –applications of AAS.

UNIT III

ELECTROANALYTICAL TECHNIQUES: Polarography – Theory, apparatus ,DME, diffusion, kinetic and catalytic currents, current voltage curves for reversible and irreversible systems, qualitative and quantitative applications to inorganic systems. Amperometric titrations – Theory, apparatus, types of titration curves, successive titrations and two indicator electrodes , applications – Complexometric titrations –chelating agents, types of EDTA titration – direct and back titrations, replacement titrations – masking and demasking reagents.

UNIT IV

SEPARATION METHODS - I: Normal and Reversed-phase liquid chromatography – Theory and applications – HPLC– principle, instrumentation, apparatus and materials,

column efficiency and selectivity , applications – GC chromatography – principle, instrumentation, retention volume, resolution and applications.

UNIT V

SEPARATION METHODS – II: Gel chromatography or Gel Permeation Chromatography – Principle, Materials, Gel preparation, column Packing and Detectors – applications and advantages of gel chromatography.Ion Exchange Chromatography – Definition, Principle, cation and anion exchangers –regeneration - column used in separations - Ion exchange capacity and techniques –Applications.

References:

1. R.Wiesendanger, scanning probe microscopy and spectroscopy, Cambridge university press, 1994
2. Frank A.Settle, Handbook of instrumental techniques for analytical chemistry, Prince Hall ,Newjersey,1997
3. Gurdeep R. Chatwal, Sham K. Anand, Instrumental methods of chemical analysis, Himalaya Publishing House,2011
4. P.Atkins and J.de paulaatkins, Physical chemistry, 8th Ed., Oxford university Press, Newdelhi, 2008
5. F.scholz, Electroanalytical methods, Springer,2ndEd.,2010.

CORE COURSE – XV PROJECT / DISSERTATION WITH VIVA VOCE

Objectives: To promote original thinking, insemination of knowledge, modulation and innovation of thought, as an exercise, in order to transport the young minds to the expanding horizon of their chosen area of knowledge and transform them into knowledge generators.

Project / Dissertation	**80 Marks**
2 Reviews	20+20 = 40marks
Report Valuation	40 Marks
Viva voce	**20 Marks**