

## J.J COLLEGE OF ARTS AND SCIENCE (Autonomous)

NAAC Re-Accredited With Grade 'A'  
SIVAPURAM, PUDUKKOTTAI-622422

### DEPARTMENT OF CHEMISTRY PG-PROGRAMME-CHEMISTRY

Course Structure under CBCS Autonomous Status  
For Candidate Admitted from the Academic year **2016-2017**

Sem	Course Code	Course Title	Hrs/ Week	Credit	Exam Hrs	Marks		Total
						Int	Ext	
<b>I</b>	P1RCHCC1	Organic Chemistry I	6	5	3	25	75	100
	P1RCHCC2	Inorganic Chemistry I	6	5	3	25	75	100
	P1RCHCC3P	Organic Chemistry Practical-I	6	5	6	40	60	100
	P1RCHCC4P	Inorganic Chemistry Practical-I	6	5	6	40	60	100
	P1RCHEC1	Bioorganic Chemistry/ Medicinal Chemistry	6	3	3	25	75	100
	<b>Total</b>			<b>30</b>	<b>23</b>			
<b>II</b>	P2RCHCC5	Physical Chemistry-I	5	5	3	25	75	100
	P2RCHCC6	Physical Methods in Chemistry-I	5	5	3	25	75	100
	P2RCHCC7	Organic Chemistry-II	5	5	3	25	75	100
	P2RCHCC8P	Organic Chemistry Practical-II	5	5	6	40	60	100
	P2RCHCC9P	Inorganic Chemistry Practical-II	5	5	6	40	60	100
	P2RCHEC2	Industrial Chemistry/ Green Chemistry	5	3	3	25	75	100
	<b>Total</b>			<b>30</b>	<b>28</b>			
<b>III</b>	P3RCHCC10	Physical Chemistry-II	5	5	3	25	75	100
	P3RCHCC11	Inorganic Chemistry-II	5	5	3	25	75	100
	P3RCHCC12	Physical Methods in Chemistry-II	5	5	3	25	75	100
	P3RCHCC13P	Physical Chemistry Practical-I	5	5	6	40	60	100
	P3RCHCC14P	Physical Chemistry Practical-II	5	5	6	40	60	100
	P3RCHEC3	Supramolecular chemistry and CrystalEngineering/ Natural Products	5	3	3	25	75	100
	<b>Total</b>			<b>30</b>	<b>28</b>			
<b>IV</b>	P4RCHEC4	Analytical Chemistry/ Advanced Topics in Chemistry	6	3	3	25	75	100
	P4RCHCC15PW	Project Work	24	8	3			100
	<b>Total</b>			<b>30</b>	<b>11</b>			
<b>Grand Total</b>			<b>120</b>	<b>90</b>				<b>1900</b>

CC-Core course/EC-Elective Course/P-Practical

**SEMESTER-I: CORE COURSE-I: ORGANIC CHEMISTRY-I**

**Course Code : P1RCHCC1**

**Max. Marks : 100**

**Hours/Week : 6**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To the nomenclature, structure and bonding of organic compounds*
- ❖ *To study the aromaticity and heterocyclic compounds*
- ❖ *To understand basic concepts of stereochemistry and organic photochemistry*
- ❖ *To understand the reactive intermediates and reaction mechanisms*

**UNIT – I: Nomenclature, Structure and Bonding**

**Nomenclature:** IUPAC nomenclature of linear and branched alkanes, alkenes, polyenes and alkynes with and without functional groups. Nomenclature of alicyclic, bicyclic and tricyclic compounds. (Basic skeletal structures only with or without one substituent).

**Structure and Bonding:** Localized Chemical Bonding: Electronic Structure of molecules; VB, MO and HOMO-LUMO theory, Electronegativity, Dipole Moment, Inductive and Field Effects. Bond distances, Bond angles, Bond energies. Delocalized Chemical Bonding: Bond energies and Bond distances in compounds containing delocalized Bonds, Cross conjugation, Resonance, Steric inhibition of resonance, Hyperconjugation, Keto – Enol Tautomerism.

**UNIT – II: Aromaticity and Heterocycles:**

**Aromaticity:** Concept of Aromaticity- Huckel's theory of aromaticity Five, six, seven-, and eight-membered rings - Other systems with aromatic sextets - Concept of homo-aromaticity and anti-aromaticity, Electron occupancy in MO's and aromaticity - NMR concept of aromaticity and anti-aromaticity, systems with 2,4,8 and 10 electrons, systems of more than 10 electrons, alternant and non-alternant hydrocarbons (azulene type). Bonding properties of systems with  $(4n+2)\pi$  electrons and  $4n\pi$  electrons, Heteroaromatic molecules. Annulenes and sydnones and fullerenes.

**Heterocycles:** Nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Synthesis, reactivity and applications of the following heterocycles: Pyrazoles, Oxazoles, Pyridazines, Pyrimidine and Pyrazines.

### UNIT- III: Stereochemistry

**Fundamentals of Organic Stereochemistry:** Stereoisomerism-Optical isomerism, Optical activity and chirality – Types of molecules exhibiting optical activity-Symmetry elements – Definitions – Conventions used in stereochemistry: Fischer notations, Newman, Sawhorse projection and their interconversions. Relative Configuration (D/L). Absolute configuration (R/S) - Cahn–Ingold–Prelog rules for cyclic and acyclic compounds. Atropisomerism – Biphenyls, allenes and spiranes. Enantiomerism of compounds containing chiral heteroatoms – Walden inversion – Asymmetric synthesis based on Cram's rule and Prelog's rule. Concepts of prochirality and enantiotopic and diastereotopic atoms.

**Geometrical Isomerism:** E & Z, Syn and anti nomenclature, determination of configuration of geometrical isomers, stereospecific and stereoselective reactions – [elementary examples].

**Conformational Analysis:** Basic concepts of conformational analysis – conformations of *n*-butane, cyclohexane and decalins.

### UNIT-IV: Reactive Intermediates and Reaction Mechanisms

**Reactive Intermediates:** Carbocations, carbanions, carbenes, nitrenes and arynes – generation and stability. Correlation of reactivity with structure of reactive intermediates. Free radicals – configurations – identification by chemical and spectral methods – free radical halogenation - NBS.

**Methods of Determining Reaction Mechanisms:** Types of reactions: homolytic and heterolytic cleavages of bonds, characteristics of nucleophilic, electrophilic and free radical reactions. thermodynamic and kinetic aspects, Hammond's postulate, isotope effects. Energy profile diagrams–intermediate versus transition state, product analysis and its importance, crossover experiments, kinetic methods, stereochemical studies, isotopic and substituent effects.

### UNIT- V: Organic Photochemistry

**Organic Photochemistry:** Fundamental concepts – Jablonski diagram – energy transfer, characteristics of photoreactions, photoreduction and photooxidation, photoreactions of ketones and enones, Norrish Type I and II reactions. Photochemistry of alkenes, dienes and aromatic compounds, reactions of unactivated centres – photolytic cycloadditions and photolytic rearrangements – photosensitisation – photoadditions – Barton reaction – ParternoBuchi reaction.

**Text Books**

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 5<sup>th</sup>Ed., Wiley, 2000.
2. D. Nasipuri, Stereochemistry of organic compounds-Principles and applications, New Age International, 2<sup>nd</sup>Ed, 2002.
3. R.K. Bansal, Organic Reaction Mechanisms, Tata McGraw Hill, 1975.
4. P.S. Kalsi, Stereochemistry, Wiley eastern limited, New Delhi, 1990.
5. G.R. Chatwal, Organic Photochemistry, Himalaya Publications house, 1<sup>st</sup>Ed, 1998.

**Reference Books**

1. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6<sup>th</sup>Ed., Pearson, 1992.
2. F.A. Carey and R.J. Sundberg –“Advanced organic chemistry” Vol. A and B–5<sup>th</sup>Ed., 2007.
3. I.L. Finar, Organic Chemistry, Vol.II, 5<sup>th</sup>Ed., ELBS 1975.
4. J.D. Coyle, Organic Photochemistry - Wiley, 1985.
5. J.M. Coxon, B. Halton, Organic Photochemistry, Camb. Uni. Press, 2<sup>nd</sup>Ed, 1987.
6. Peter Sykes, A Guide Book of Reaction Mechanism, 5<sup>th</sup>Ed., 2005.

**SEMESTER-I: CORE COURSE-II: INORGANIC CHEMISTRY-I**

**Course Code : P1RCHCC2**

**Max. Marks : 100**

**Hours/Week : 6**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To make students understand the chemistry of main group elements and its compounds*
- ❖ *To know the stability and theory of coordination compounds*
- ❖ *To understand the reaction mechanism of coordination compounds and inorganic photochemistry*

**UNIT – I: Main Group Chemistry and Ionic Model**

Chemistry of boron–borane, higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon–silanes, higher silanes, multiple bonded systems, disilanes, silicon nitrides, siloxanes and silicates. P-N compounds, cyclophosphazenes and cyclophosphazanes. S-N compounds –  $S_4N_4$ ,  $(SN)_x$ .

**Ionic Model:** Lattice energy – Born-Landé equation – Kapustinski equation – high  $T_c$  superconductors – solid state reactions – types and examples.

**UNIT-II: Coordination Chemistry: Principles**

Studies of coordination compounds in solution – detection of complex formation in solution – stability constants – stepwise and over-all formation constants – simple methods (potentiometric, pH metric and photometric methods) of determining the formation constants - factors affecting stability – statistical and chelate effects – forced configurations.

**UNIT-III: Theories of Metal - Ligand bond**

VB theory and its limitations – crystal field theory – splitting of  $d$ -orbitals under various geometries – factors affecting splitting – CFSE and evidences for CFSE (Structural and thermodynamic effects) – spectrochemical series – Jahn-Teller distortion – spectral and magnetic properties of complexes – site preferences - limitations of CFT – ligand field theory – MO theory –  $\sigma$ (sigma) – and  $\pi$ (pi) – bonding in complexes – Nephelauxetic effect – the angular overlap model.

**UNIT – IV: Coordination Chemistry – Reaction Mechanism**

Kinetics and mechanism of reactions in solution – labile and inert-complexes – ligand displacement

reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions – trans effect – theory and applications. Electron transfer reactions – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes. Application of electron transfer reactions in inorganic–isomerisation and racemisation reactions of complexes. Molecular rearrangement – reactions of four and six-coordinate complexes – interconversion between stereoisomers. Reactions of coordinated ligands – template effect and its application for the synthesis of macrocyclic ligands – unique properties.

### **UNIT – V: Inorganic Photochemistry**

Electronic transitions in metal complexes, metal-centered and charge-transfer transitions – 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 rules, photoactive excited states, V-C model–photophysics and photochemistry of ruthenium–polypyridine complexes, emission and redox properties – photochemistry of organometallic compounds, metal carbonyl compounds, compounds with metal-metal bonding Reinecke's salt chemical actinometer.

### **Text Books**

1. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 4<sup>th</sup>Ed., A Wiley - Interscience Publication, John –Wiley & Sons, USA.
2. J.E. Huheey, Inorganic Chemistry 3<sup>rd</sup> Ed., Harper & Row publisher, Singapore.
3. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, 1996.
4. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley, New York, 1988.

### **Reference Books**

1. M. C. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd. 2<sup>nd</sup>Ed., 1985.
2. A. W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, New York, 1975.
3. F. Basolo and R.G. Pearson, Mechanism of Inorganic Reactions, John Wiley, New York.

**SEMESTER-I: CORE COURSE-III: ORGANIC CHEMISTRY PRACTICAL -1**

**Course Code :P1RCHCC3P**

**Max. Marks : 100**

**Hours/Week : 6**

**InternalMarks : 40**

**Credit : 5**

**External Marks : 60**

**Objectives**

- ❖ *To learn the separation of binary organic mixtures*
- ❖ *To learn the methods of qualitative analysis of organic compounds*
- ❖ *To learn some single stage preparation of organic compounds*

**A. Qualitative Analysis of an organic mixture containing two components.**

Pilot separation, bulk separation, analysis, and derivatization.

**B. Preparation of Organic compounds.(Single stage).**

- (a) methyl *m*- nitrobenzoate from methylbenzoate (nitration)
- (b) glucose pentaacetate from glucose (acetylation)
- (c) resorcinol from resorcinol (acetylation)
- (d) benzophenoneoxime from benzophenone (addition)
- (e) *o*-chlorobenzoic acid from anthranilic acid (Sandmeyer reaction)
- (f) *p*-benzoquinone from hydroquinone (oxidation)
- (g) Phenyl-azo-2-naphthol from aniline (diazotization)

**Reference Book**

1. B.S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, Vogel's Textbook of Practical Organic Chemistry- 5<sup>th</sup> Ed., Pearson publication.
2. V. Vengataswaran,*et al.*, Basic Principle of Practical Chemistry – Sultan Chand and sons, New Delhi (1997).
3. Ganapragasm and Ramamurthy, Organic Chemistry Lab Manual, 2<sup>nd</sup> Ed., S. Vishwanathan Printers and Publishers (P) Ltd., Chennai (2007)

**SEMESTER-I: CORE COURSE-IV: INORGANIC CHEMISTRY PRACTICAL -1**

Course Code :P1RCHCC4P

Max. Marks : 100

Hours/Week : 6

Internal Marks : 40

Credit : 5

External Marks : 60

**Objectives**

- ❖ *To learn the qualitative analysis of common metals and rare metals*
- ❖ *To learn colorimetric analysis*
- ❖ *To learn to prepare inorganic complexes*

**1. Theoretical Principles**

Classification of cations into groups, group reagents – intergroup and intragroup separations –Confirmatory test for cations– the reactions and the products.

**2. Analysis of Mixture of Cations**

Analysis of a mixture of four cations containing two common and two rare cations.

**Common cations:** Group I: Pb and Hg; Group II: Hg, Cu, Cd, Bi, Sb, As, and Sn; Group III: Al, Fe, and Cr; Group IV: Mn, Zn, Co, and Ni; Group V: Ca, Sr, and Ba; Group VI: Mg, K, and  $\text{NH}_4^+$ .

**Rare cations:** Group I: W and Tl; Group IA: Se and Te; Group II: Mo; Group III: Be, Tl, Ce, Ti, Th, Zr, V, and U; Group VI : Li

**3. Estimation of ions using photoelectric colorimeter.**

Estimation of Cu, Fe, Ni, Cr and Mn using photoelectric colorimeter.

**Reference Books**

1. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis, 3<sup>rd</sup> Ed., The National Publishing Company, Chennai, 1990.
2. Vogel's Text book of Inorganic Qualitative Analysis, 7<sup>th</sup> Ed, ELBS, London, 1996.
3. G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, Vogel's 's Textbook of Quantitative Chemical Analysis; 5<sup>th</sup> Ed., VELBS" 1989.
4. J. D. Woollins, Ed., Inorganic Experiments; VCH: Weinheim, 1994.



**SEMESTER-I: ELECTIVE COURSE-I: BIOORGANIC CHEMISTRY**

**Course Code :PIRCHEC1**

**Max. Marks : 100**

**Hours/Week : 6**

**Internal Marks : 25**

**Credit : 3**

**External Marks : 75**

**Objectives**

- ❖ *To understand amino acids and proteins*
- ❖ *To know enzyme and co-factors*
- ❖ *To understand nucleic acids and protein synthesis*
- ❖ *To understand planning of organic synthesis*

**UNIT-I: Amino Acids and Proteins**

**Amino Acids:** Structure, classification, synthesis and properties of amino acids, isoelectric point, biosynthesis of amino acids. Peptides: oligo- and polypeptides, geometry of peptide linkage, N-terminal and C-terminal residue analysis, synthesis of peptides-amino and carboxyl protecting groups-solid phase peptide synthesis.

**Proteins:** classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins, collagen and triple helix.

**UNIT-II: Enzymes and Cofactors**

**Enzymes:** Mechanism of enzyme catalysis, Factors influencing enzyme action, Examples of typical enzyme mechanisms: chymotrypsin, ribonuclease and lysozyme, Enzyme-catalyzed addition, elimination, condensation, carboxylation and decarboxylation, isomerisation, group transfer and rearrangement reactions.

**Co-factors:** structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, lipoic acid and Vitamin B<sub>12</sub>. Mechanisms of reactions catalysed by the above cofactors.

**UNIT-III: Nucleic Acids and Protein Synthesis**

**Nucleic Acids:** Nucleotides and nucleosides, DNA: primary and secondary structure-replication of DNA.

**RNA and Protein Synthesis:** Messenger RNA synthesis-transcription, Ribosomes- rRNA, Transfer RNA. Determination of base sequence of DNA. Polymerase Chain Reaction (PCR).

Antisense technology in chemotherapy and other nucleic acid-targeted drugs-intercalaters, sequence specific drugs. A brief account of ribozyme and iRNA( interference).

#### **UNIT-IV: Lipids and Carbohydrates**

**Lipids:**Classification – Neutral lipids,phospholipids(lecithines,cephalins,plasmalogens) and glycolipids-importance,synthesis and degradation.Bio-synthesis of cholesterol,lipids-synthesis of fatty acids and triglycerids

**Carbohydrates:** Classification – reducing and non-reducing sugar.Glucose:structure,conformation,stability. Carbohydrates of cell membrane – starch,cellulose and glycogen,TCAcycle.Relation between glycolysis and respiration.principles of bioenergetics.

#### **UNIT-V: Planning of organic synthesis**

Designing organic synthesis-disconnection approach-synthons and synthetic equivalents-one group disconnections: alcohol, olefin, ketone, acids-two group disconnections:1,2, 1,3, 1,4 and 1,5-difunctional compounds-convergent synthesis-functional group interconversions- functional group additions-carbonheteroatom bonds-methods for 3- to 6-membered rings.

#### **Text Books**

1. Hermann Dugas and C. Penny, Springe-Verlag.,Bioorganic Chemistry: A Chemical approach to Enzyme action.
2. N.C. Price and L.Stevens, Fundamentals of Enzymology, Oxford University Press.
3. C. Walsh, W.H.Freeman., Enzymatic Reaction Mechanisms,
4. Stuart Warren, Designing Organic Synthesis: The Disconnection Approach, Wiley, 2<sup>nd</sup> Ed., 1984.

#### **References Books**

1. H. B. Kagan, Asymmetric Synthesis, Thieme Medical Publishers, 2003.
2. Francis A. Carey and Richard B. Sundberg, Advanced Organic Chemistry: Part-A and Part-B by, Springer, 5<sup>th</sup>Ed, 2007.

**SEMESTER-I: ELECTIVE COURSE-I: MEDICINAL CHEMISTRY**

Course Code :PIRCHEC1

Max. Marks : 100

Hours/Week : 6

Internal Marks : 25

Credit : 3

External Marks : 75

**Objectives**

- ❖ *To understand Drugs and Their Mechanism of Action*
- ❖ *To understand Drug Discovery, Design and Development*
- ❖ *To know Lead and analogue synthesis*

**UNIT-I: Introduction to Drugs and Their Action**

**Drugs:** Historical background-sources and classification of drugs-important terminologies in medicinal chemistry. **Drug Action:** Role of intermolecular forces-drug targets: lipids, carbohydrates, proteins (enzymes,receptor) and nucleic acids as drug targets. Pharmacokinetics and pharmacodynamics: administration,absorption, distribution, metabolism, elimination of drugs-bioavailability of drugs-side effects.

**UNIT-II: Selected Examples of Drugs and Their Mechanism of Action**

**Antibacterial agents:** Mechanism of action-antibacterial agents that act against cell metabolism(sulfonamides), inhibit cell wall synthesis (penicillins, cephalosporins), interact with plasma membrane(valinomycin and gramicidin A), impair protein synthesis (tetracyclines, chloramphenicol) and act on nucleicacids (quinolones and fluoroquinolones, rifamycins).

**Antiviral and antifungal agents:** General principles-nucleic acidsynthesis inhibitors (HIV), host cell penetration inhibitors, inhibitors of viral protein synthesis. Azoles, allyamines and phenols. Anticancer drugs and their mechanism of action- role of antimetabolites, antisense drugs, alkylating agents and interchelating agents in cancer chemotherapy.

**Cardiovascular drugs:** Antiarrhythmic and antihypertension drugs.

**UNIT-III: Drug Discovery, Design and Development**

Identification of diseases and corresponding targets, bioassays and leads. Stereochemistry and solubilityissues in drug design. Structure activity relationships (SARs): changing size and shape-introduction of newsubstituents. Quantitative structure activity relationships (QSARs): lipophilicity-electronic and steric effects-Hansch Analysis-Topliss decision tree. Chemical and process development of drugs. Preclinical trials:pharmacology, toxicology, metabolism and

stability studies-formulation. Clinical trials: phase I-IV studies ethical issues. Patent protection.  
Regulation

#### **UNIT-IV: Lead and Analogue Synthesis-I**

**Designing organic synthesis:** Disconnection approach-synthons and synthetic equivalents-one group disconnections: alcohol, olefin, ketone, acids-two group disconnections: 1,2-, 1,3-, 1,4- and 1,5-difunctional compounds-convergent synthesis-functional group interconversions- functional group additions-carbon heteroatom bonds-methods for 3- to 6-membered rings.

#### **UNIT-V: Lead and Analogue Synthesis-II**

**Combinatorial synthesis in medicinal chemistry:** Solid phase techniques-methods of parallel synthesis-mix and split techniques-dynamic combinatorial chemistry-screening and deconvolution-limitations of combinatorial synthesis. Asymmetric synthesis: basic principles-stereoselective and stereospecific reactions- methods for determining enantiomeric excess-chiral auxiliary, reagents and catalysts and their applications (wherever applicable) in alkylation, hydrogenation, hydroxylation, epoxidation and hydroboration of alkenes, reduction of ketones-Cram and Felkin-ahn models. Noyori's BINAP – Jacobson catalyst – Evans catalyst.

#### **Text Books**

1. Gareth Thomas, Fundamentals of Medicinal Chemistry, John Wiley & Sons, 2003.
2. Gareth Thomas, Medicinal Chemistry: An Introduction, Wiley-Interscience, 2<sup>nd</sup> Ed, 2008.
3. Graham L. Patric, An introduction to Medicinal Chemistry, Oxford University Press, USA, 3<sup>rd</sup> Ed., 2005.
4. Wilson and Giswald's Textbook of Organic Medicinal and Pharmaceutical Chemistry by John Block and John M Beale (Eds), Lippincott Williams & Wilkins, 11<sup>th</sup> Ed., 2003.

#### **Reference Books**

1. The Organic Chemistry of Drug Design and Drug Action by Richard B. Silverman, Academic press, 2<sup>nd</sup> Ed., 2004.
2. Designing Organic Synthesis: The Disconnection Approach by Stuart Warren, Wiley, 2<sup>nd</sup> Ed., 1984.
3. Asymmetric Synthesis by H. B. Kagan, Thieme Medical Publishers, 2003.
4. Francis A. Carey and Richard B. Sundberg, Advanced Organic Chemistry: Part-A and Part-B, Springer, 5<sup>th</sup> Ed., 2007.

**SEMESTER-II: CORE COURSE-V: PHYSICAL CHEMISTRY –I**

**Course Code :P2RCHCC5**

**Max. Marks : 100**

**Hours/Week : 5**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To understand Group theory, Quantum Mechanics and Chemical Kinetics*
- ❖ *To know Photochemistry and Solar cells*
- ❖ *To understand the Molecular Thermodynamics*

**UNIT – I: Quantum Mechanics**

Inadequacy of classical mechanics, Black body radiation, Planck's quantum concept, Photoelectric effect. Bohr's theory of hydrogen atom: Hydrogen spectra, Wave-particle dualism, Uncertainty principle, Inadequacy of old quantum theory. Schrödinger equation, Postulatory basis of quantum mechanics. Operator algebra: operator, linear and hermitian, eigen functions and eigen values, angular momentum operator, commutation relations, related theorems. Applications of wave mechanics to simple systems – particle in a box, one and three-dimensional, distortion of the box and Jahn-Teller effect, quantum numbers, zero-point energy, orthogonalisation and normality, finite potential barrier – tunneling.

**UNIT – II: Chemical Kinetics- I**

Theories of reaction rate – Absolute reaction rate theory (ARRT) - Significance of reaction coordinate – Potential energy surfaces – Kinetic isotope effect – Molecular dynamics – Marcus theory of electron transfer processes. Principle of microscopic reversibility-Steady-state approximation – Chain reactions: thermal and photochemical reactions between hydrogen and halogens - Explosions and hydrogen – oxygen reactions. Application of ARRT to solution kinetics-effect of solvent and ionic strength, influence of pressure on rates in solution.

**UNIT – III: Group theory - Concepts**

Elements of group theory – definition – group multiplication tables – conjugate classes, conjugate and normal subgroups – symmetry elements and operations – point groups – assignment of point groups to molecules, - Matrix representation of geometric transformation and point groups – reducible and irreducible representations– properties of irreducible representation – construction of character tables – bases for irreducible representation – direct product – symmetry adapted linear combinations – projection operators.

#### **UNIT –IV: Photochemistry and Radiation Chemistry**

**Photochemistry:**Chemi-luminescens, phosphorescences, quantum yield. Photo-physical processes electronically excited molecules Jablonski diagram – Stern-Volmer equation and its applications – experimental techniques in photochemistry – chemical action meters –lasers and their applications.

**Photo-catalysts and photovoltaiccell:**Solar energy: Conversion, Basic concept of photo-catalyst, visible light water splitting, photovoltaic cells. Perovskites solar cells. Dye sensitized solar cells, efficiency and measurement.

**Fast reaction techniques:** Introduction, flow methods (continuous and stopped flow methods)- Relaxation methods (T and P jump methods) – Pulse techniques (pulse radiolysis, flash photolysis, Shock tube method)- molecular beam method – lifetime method.

#### **UNIT – V: Molecular Thermodynamics -I**

Calculation of Thermodynamic probability of a system – Difference between thermodynamic probability and statistical probability – Ergodic hypothesis –Derivation of Boltzman distribution equation – physical significance of partition function- translational, rotational, vibrational and electronic partition functions – Quantum statistics – Bose – Einstein and Fermi – Dirac distribution equations – comparison of B.E and F.D statistics with Boltzman statistics – Concept of Negative Kelvin Temperature.Relationships between partition function and thermodynamic properties such as  $E$ ,  $H$ ,  $C_p$ ,  $C_v$ ,  $P$ . Derivation of  $PV=RT$ , Molecular interpretation of entropy- Derivation of  $S=k\ln W$ - Establishment of analogous nature of  $S= k\ln W$  to  $ds= dq_{rev}/T$ . Calculation of  $S$ ,  $A$ ,  $G$  etc., from partition functions– calculation of equilibrium constants for very simple reactions.

#### **Text Books**

1. F. Albert Cotton, Chemical Applications of Group Theory, 3<sup>rd</sup>Ed., John Wiley & Sons,2003
2. K.J. Laidler, Chemical Kinetics, 2<sup>nd</sup>Ed., Tata McGraw Hill, 1975.
3. P.W. Atkins,Physical Chemistry, 7<sup>th</sup> Ed., Oxford University press, 2002.
4. R.P.Wayne, Photochemistry, Butterworths,London, 1970.
5. J. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, ShobhanLalNagin, New Delhi, 1981.

#### **Reference Books:**

1. Robert L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, Inc., 1998.
2. D. A.McQuarrie and D. Simon, Physical chemistry, A Molecular Approach, Viva Books.
3. A.K. Chandra, Introductory Quantum Chemistry, 4<sup>th</sup>Ed., Tata McGraw Hill,1994.
4. R.K. Prasad, Quantum Chemistry, New Age International Publishers, New Delhi, 1997.

**SEMESTER-II: CORE COURSE-VI: PHYSICAL METHODS IN CHEMISTRY-I**

**Course Code :P2RCHCC6**

**Max. Marks : 100**

**Hours/Week : 5**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To understand the Principles of Molecular Spectroscopy*
- ❖ *To understand NMR,UV-Visible,IR Spectroscopy*
- ❖ *To know ESR, ORD,CD and X-Ray Diffraction*

**UNIT-I: Principles of Molecular Spectroscopy**

Interaction of electromagnetic radiation with molecular systems – Time evolution of the systems under radiation – Einstein transition probability for induced absorption and spontaneous and stimulated emission – Transition moment and Oscillator strength Microwave spectroscopy – rotational spectra of diatomic molecules, rigid and non-rigid rotors, - Intensity of spectral lines, - Effects of isotopic substitution – Microwave spectra of polyatomic molecules – Linear and symmetric top molecules, Infrared spectra – diatomic molecules, simple harmonic and anharmonic oscillators, - diatomic vibrating rotator, rotation-vibration spectrum of carbon monoxide, - Interaction of rotation and vibration (breakdown of Born – Oppenheimer approximation) – Influence of the rotation on the spectrum of polyatomic molecules, linear and symmetric top molecules, parallel and perpendicular vibrations, Influence of nuclear spin. Raman spectra – Rotational Raman spectra of linear and symmetric top molecules – Vibrational Raman spectra, Rotational fine structure. Electronic spectra of diatomic molecules, - Vibrational coarse structure – Intensity of vibrational lines in electronic spectra – Rotational fine structure – Fortratdiagram.

**UNIT-II:Advanced Spectroscopy (NMR)**

**<sup>1</sup>H NMR:** Multiplicity – Coupling constant – First order and second order proton, Spin - spin splitting – Dependence of  $J$  on dihedral angle –Vicinal and geminal coupling constants – Karplus equation – long range coupling constants, Influence of stereochemical factors on chemical shift of protons. Simplification of complex spectra – Double resonance techniques, shifts reagents. Chemical spindecoupling of rapidly exchangeable protons (OH, SH, COOH, NH, NH<sub>2</sub>), an elementary treatment of NOE phenomenon. **<sup>13</sup>C NMR:** Basic theory of FT – NMR, Relaxation – Broad band decoupling. Off resonance decoupling and chemical shifts of common functional

groups, DEPT spectra. Identification of small compounds based on NMR data. 2D Techniques:  $^1\text{H}$ - $^1\text{H}$  COSY,  $^1\text{H}$ - $^{13}\text{C}$  COSY-HMBC and NOESY.

### **UNIT-III: Advanced Spectroscopy: (UV –Vis, IR)**

**UV-Visible Spectroscopy** : Introduction - Instrumentation, Sampling techniques - Woodward-Fieser and Scott rules for conjugated dienes and polymers, ketones, aldehydes,  $\alpha$  and  $\beta$ -unsaturated acids, esters, nitriles, and amides. Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives - Study of steric effect in aromaticity.

**Infrared Spectroscopy**: Introduction- Instrumentation, Sampling techniques, factors influencing group frequencies – Both internal and external – quantitative studies. Hydrogen bonding – (intermolecular and intramolecular).

### **UNIT: IV: ESR, ORD and CD**

**Electron Spin Resonance Spectroscopy**: Basic principles – comparison between ESR and NMR spectra – hyperfine splitting – factors affecting the magnitude of  $g$  – values – calculation of unpaired electron density on an atom in a delocalized system – applications to organic free radicals. **Optical Rotatory Dispersion and Circular Dichroism**: Introduction to theory and terminology – Cotton effect – ORD curves – axial haloketone rule and its applications – octant rule – its applications – applications of ORD to determine absolute configuration of monocyclic ketones – comparison between ORD and CD – their inter relationships. **Mass Spectrometry**: Instrumentation – Resolution, EI and CI methods – Base peak, isotopic peaks, metastable peak, parent peak, determination and use of molecular formula, recognition of molecular ion peak – FAB. Fragmentation – General rules – Pattern of fragmentation for various classes of compounds, McLafferty rearrangement, Importance of metastable peaks.

### **UNIT-V: Methods of Diffraction**

**X-ray diffraction**: X-ray diffraction by single crystal – Space groups – Systematic absences in X-ray data and identification of lattice types, glide planes and screw axes. X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Structure solution by Heavy atom method and direct method. Determination of absolute configuration of molecules. A brief account of Cambridge Structural Database (CSD) and Protein Data Bank (PDB). **Electron Diffraction by gases**: Scattering intensity vs Scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. **Neutron**



**diffraction by crystals:** Magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

**Text Books**

1. C.N. Banwell, Fundamentals of molecular Spectroscopy, 3<sup>rd</sup> Ed., TMH, New Delhi, 1983.
2. P.K.Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley New York, 1989.
3. W. Kemp, Organic Spectroscopy, 3<sup>rd</sup> Ed., MacMillon, 1994.
4. Y.R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical applications, S.Chand, 1992.
5. W.Clegg, Crystal structure determination, Oxford University press, New York, 1998.
6. G.H.Stout, L.H. Jensen, X-ray structure determination: A practical guide, John wiley & sons Publication: New York, 1989.

**Reference Books:**

1. B.P. Straughan and S.Walker Spectroscopy Vol.3, Chapman Hall London, 1976.
2. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1964.
3. P.M. Silverstein, F. X. Wester, Spectroscopic Identification of Organic Compounds, 6<sup>th</sup> Ed., Wiley 1998.
4. J.R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall, 1965.
5. J.P. Glusker, K. N. Trueblood, Crystal structure analysis: A primer., Oxford university press, New York, 1972.

**Webpages:**

1. Cambridge Structural Database (CSD) - <http://www.ccdc.cam.ac.uk/products/csd/>
2. Protein Data Bank (PDB) - <http://www.rcsb.org/pdb/home/home.do>

**SEMESTER-II: CORE COURSE-VII: ORGANIC CHEMISTRY -II**

**Course Code :P2RCHCC7**

**Max. Marks : 100**

**Hours/Week : 5**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To understand the Nucleophilic and Electrophilic Substitution Reactions*
- ❖ *To know about Addition and Elimination Reactions*
- ❖ *To understand the Pericyclic Reactions and Rearrangements*
- ❖ *To know the Some important Reagents in Organic Synthesis*

**UNIT – I: Nucleophilic Substitution Reactions**

Aliphatic Nucleophilic substitution: Mechanisms–Effect of structure–Stereochemical factors–Neighbouring group participation, substitutions at allylic and vinylic carbons. Correlation of structure with activity–Solvent effects.Rearrangements involving Carbocations-Wagner Meerwein and Dienone–phenol rearrangements.Aromatic Nucleophilic substitution: $S_N1$ ,  $S_NAr$ , Benzyne mechanism–reactivity orientation–Ullman, Sandmeyer and Chichibabin reaction.Rearrangements involving nucleophilic substitution–Stevens–sommelet Hauser and Von– Richter rearrangements.

**UNIT - II: Electrophilic Substitution Reactions**

**Aromatic electrophilic substitution reaction:**Orientation, reactivity and mechanisms based on transition state theory with suitable reactions, substitutions in Thiophene, Pyridine and Pyridine-N-Oxide. Quantitative treatment of the structural effects on reactivity. Substituents effects – Origins of Hammett equation–Principles of Hammett correlation – Effect of structure on reaction mechanisms Hammett parameters;  $\sigma$  and  $\rho$ , modified forms of Hammett equation. Taft Equation.Aliphatic Electrophilic Substitution:  $S_E2$ ,  $S_{Ei}$  and  $S_{E1}$  mechanisms, Diazonium coupling reactions. Metals as electrophile in substitution reactions and decomposition of diazonium salts.

**UNIT – III: Addition and Elimination Reactions**

**Addition Reactions:** Addition to carbon–carbon multiple bonds: Electrophilic, nucleophilic and free radical additions–Orientation of the addition–Stereochemical factors influencing the addition of bromine and hydrogen bromide, hydroxylation, hydroboration leading to formation of alcohols. Addition to carbonyl and conjugated carbonyl systems-Mechanism–Grignard reagents–1,2 and 1,4-additions(dimethyl lithium cuprate), Benzoin, Knoevenagel, Stobbe and

Darzen's glycidic ester condensation and Reformatsky reactions. **Elimination Reactions:** Mechanisms; E1, E2, E1cB – Stereochemistry of elimination, Hofmann and Saytzeff rules – Competition between elimination and substitution - Pyrolytic *cis* elimination, Chugaev reaction – Examples such as dehydration, dehydrohalogenation, Hofmann degradation, Cope elimination – Bredt's rules with examples.

#### UNIT – IV: Pericyclic Reactions and Rearrangements

Concerted reactions – stereochemistry – orbital symmetry and concerted symmetry and correlation diagram – Frontier molecular orbital approach – Woodward and Hoffmann rules – Electrocyclic reactions – cycloaddition reactions – sigmatropic rearrangements – selection rules and examples with simple molecules – 1,3 and 1,5 hydrogen shifts – Cope and Claisen rearrangements. Other molecular rearrangements Wolff-Lossen-Schmidt-Favorski-Pummerer and Hofman Freytas reagents.

#### UNIT-V: Reagents in Organic Synthesis

**Reduction:** Catalytic hydrogenation – Wilkinson Catalyst, dehydrogenation, reduction with LAH, NaBH<sub>4</sub>, tertiary butoxy aluminum hydride, NaCNBH<sub>3</sub>, tributyltin hydride, alkali metals for reduction, reductions involving hydrazines, Wolf Kishner reduction. **Oxidation:** Osmium tetroxide, Sharpless asymmetric epoxidation, Chromyl chloride, Ozone, DDQ, Dioxiranes, Lead tetraacetate, Selenium dioxide, DMSO with either Ac<sub>2</sub>O or Oxalyl chloride, Dess-Martin reagent. Synthesis involving phase transfer catalysis (PTC), use of crown ethers, Merrifield resin, Baker's yeast.

#### Text Books

1. S.H. Pine, J.B. Hendrickson, D.J. Cram and G.S. Hammond, Organic chemistry, McGraw Hill, 4<sup>th</sup> Ed., 1980.
2. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, Harper and Row, 1976.
3. R.K. Bansal, Reaction Mechanism in Organic Chemistry, Tata McGraw Hill, 1990.

#### Reference Books

1. J. March, Advanced Organic Chemistry; Reactions, Mechanisms and Structure, 5<sup>th</sup> Ed., Willey, 2000.
2. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Parts A & B, Plenum, 2002.

**SEMESTER-II: CORE COURSE-VIII: ORGANIC CHEMISTRY PRATICAL-II**

Course Code :P2RCHCC8P

Max. Marks : 100

Hours/Week : 5

Internal Marks : 40

Credit : 5

External Marks : 60

**Objectives**

- ❖ *To learn quantitative analysis in organic chemistry*
- ❖ *To learn some double stage organic preparations*

**A. Quantitative analysis of organic compounds**

Estimation of phenol, aniline, ketone, glucose, nitrobenzene, saponification value of an oil and Iodine value of an oil.

**B. Preparation of organic compounds (Double stage)**

- a. *p*-bromo acetanilide from aniline (acetylation and bromination).
- b. acetyl salicylic acid from methyl salicylate (hydrolysis and acetylation).
- c. 1,3,5-tribromobenzene from aniline (bromination, diazotization and hydrolysis).
- d. *p*-nitroaniline from acetanilide (nitration and hydrolysis).
- e. benzilic acid from benzoin (rearrangement).
- f. *p*-amino benzoic acid from *p*-nitro toluene (oxidation and reduction).
- g. benzanilide from benzophenone (rearrangement).
- h. *p*-bromoaniline from acetanilide (bromination and hydrolysis).
- i. *m*-nitroaniline from nitrobenzene (nitration and reduction).
- j. 1,2,4-triacetoxy benzene from hydroquinone (oxidation and acylation).

**Text Books**

1. N.S. Gnanapragasam and G. Ramamurthy, Organic Chemistry – Lab manual, S. Viswanathan Co. Pvt. Ltd, 2007.
2. J.N. Gurtu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987.

**Reference Book**

1. Vogel's Text book of Practical Organic Chemistry, 4<sup>th</sup>Ed., ELBS/Longman, England, 1984.

**SEMESTER-II: CORE COURSE-IX: INORGANIC CHEMISTRY PRATICAL-II**

**Course Code :P2RCHCC9P**

**Max. Marks : 100**

**Hours/Week : 6**

**Internal Marks : 40**

**Credit : 5**

**External Marks : 60**

**Objectives**

- ❖ *To learn quantitative separation of metal ions in binary mixtures.*
- ❖ *To learn simple single stage preparations of some complex compounds.*

**Titrimetry and Gravimetry**

A mixture of solution(s) should be given for estimation

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

**Preparation of the Following Compounds:**

- a. Tetramminecopper (II) sulphate.
- b. Potassium trioxalatochromate (III).
- c. Potassium trioxalatoaluminate (III).
- d. Trithiourecopper (I) chloride.
- e. Trithiourecopper (I) sulphate.
- f. Dibenzyltindichloride

**Text Books**

1. G. H. Jeffery, J. Bassett, J.Mendham, R.C. Denney, Vogel's 's Textbook of Quantitative Chemical Analysis; 5<sup>th</sup> Ed., ELBS,1989.
2. J. D., Woollins, Ed., Inorganic Experiments; VCH: Weinheim, 1994.
3. G. Pass, H. Sutcliffe, Practical Inorganic Chemistry; Chapman Hall, 1965.
4. W. G. Palmer, Experimental Inorganic Chemistry; Cambridge University Press, 1954.

**SEMESTER-II: ELECTIVE COURSE-II: INDUSTRIAL CHEMISTRY**

**Course Code :P2RCHEC2**

**Max. Marks : 100**

**Hours/Week : 5**

**Internal Marks : 25**

**Credit : 3**

**External Marks : 75**

**Objectives**

- ❖ *To understand leather, dyes and fuels*
- ❖ *To know about oil,fats,soaps*
- ❖ *To know about synthetic perfumes and drugs*

**UNIT-I: Tanning of Leather and Dyes**

Introduction-Animal skin,manufacture of leather-preparation of hides-vegetable tanning-chrome tanning- finishing-oil tanning.**Dyes:**Introduction-sensation of colour-colour and constitution-nomenclature-basic operations in dyeingclassification of dyes according to the mode of application – synthesis, reaction and applications of diphenylmethane dyes-triphenylmethane dyes-phthalein dyes-xanthene dyes-acridine dyes-sulphur dyescyanine dyes.

**UNIT-II: Fuels.**

Fossil fuels- classification and unique features- Coal, Petroleum, natural gas. Biofuels: Biomass-biodiesel. Nuclear fuels: for various types of nuclear reactors. Hydrogen as fuel in the future, Hydrogen storage materials. Fuel cells – basic principle.

**UNIT-III: Oils, Fats, Waxes and Soaps**

Introduction-Distinction between oils and fats-properties and its classifications-animal fats and oilsdifference between, animal, vegetable and mineral oils-isolation of essential oils and their usesaponification value-ester value-acid value-iodide value-wijs method – Reichert meissel value-Henher value-elaident test-hydrogenation of oils – Soaps and its manufacture-general consideration in soap making – manufacture of toilet and transparent soaps – oil to be used for soap – cleansing action of soap Food chemistry: Food processing food preservatives and food additives.

**UNIT-IV: Synthetic Perfumes**

Introduction-Esters-alcohols – ketones–aionones – nitromusks – aldehydes – dipheny-production of natural perfumes-flower perfumes-fruit flavours-artificialaflavours.

## UNIT-V:Drugs

**Antibiotics:** Definition, structure- uses of chloramphenicol, ampicillin, streptomycin, tetracycline, rifamycin – Erythromycin – Properties, uses. **Sulpha drugs:** Definition and drug action of sulphadiazine, sulphapyridine, sulphathiazole and sulphafurazole. **Anesthetics:** Definition – classification – general volatile anaesthetics – ethers, nitrous oxide, chloroform, trichloro ethane, storage – advantages – disadvantages – intravenous anaesthetics: thiopental sodium, methohexitone – local anaesthetics – cocaine, procaine, benzocaine – uses – advantage – disadvantages.

### Text Books

1. Chemical Process Industries – Norrish Shreve, R. and Joseph A. Brink Jr. McGraw Hill, Industrial Book Company, London.
2. Mathew George and Lincy Joseph, Text book of pharmaceutical chemistry, 2009.
3. Jayashree Ghose – Text book of Pharmaceutical chemistry, 2<sup>nd</sup> Ed., 2003.
4. S. Lakshmi, Pharmaceutical Chemistry, 3<sup>rd</sup> Ed., Sulthan Chand and Sons, New Delhi, 2004.

### References Books:

1. Production and Properties of Industrial Chemicals – Brain A. C. S. Reinhold – New York.
2. Petroleum Products Hand Book. Guthrie V., McGraw Hill, Tokyo.
3. Industrial Chemistry (Including Chemical Engineering) – B. K. Sharma 10<sup>th</sup> Ed.,
4. Outlines of Chemical Technology – For the 21<sup>st</sup> Century – M. Gopala Rao & Matshall S. Sittig, 3<sup>rd</sup> Ed.,
5. Charles E. Carraher, Polymer chemistry, 6<sup>th</sup> Ed, Marcel Dckker, Brijbasi Art Pvt.Ltd, 2003.
6. V.R.Gowariker, N.V. Viswanathan and Jayadev Sreedhar, Polymer Science, New Age Publishers, New Delhi, 1986.

**SEMESTER-II: ELECTIVE COURSE-II: GREEN CHEMISTRY**

**Course Code :P2RCHEC2**

**Max. Marks : 100**

**Hours/Week : 5**

**Internal Marks : 25**

**Credit : 3**

**External Marks : 75**

**Objectives**

- ❖ *To understand the green chemistry*
- ❖ *To know Microwave Assisted Organic Synthesis*
- ❖ *To understand ionic liquids and Bio-Catalysts for Green Chemistry*
- ❖ *To understand alternative Reagents for synthesis*

**UNIT-I: Introduction to Green Chemistry**

Green chemistry-relevance and goals, Anastas' twelve principles of green chemistry - Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

**UNIT-II: Microwave Assisted Organic Synthesis (MAOS)**

Microwave activation – advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supports reactions – Functional group transformations – condensations reactions – oxidations – reductions reactions – multi-component reactions.

**UNIT-III: Ionic Liquids and PTC**

Introduction – synthesis of ionic liquids – physical properties – applications in alkylation – hydroformylations – epoxidations – synthesis of ethers – Friedel-craft reactions – Diels-Alder reactions – Knoevengal condensations – Wittig reactions – Phase transfer catalyst - Synthesis – applications.

**UNIT-IV: Supported Catalysts and Bio-Catalysts for Green Chemistry**

Introduction – the concept of atom economy – supported metal catalysts – mesoporous silicas – the use of Biocatalysts for green chemistry - modified bio catalysts – fermentations and biotransformations – fine chemicals by microbial fermentations – vitamins and amino acids – Baker's yeast mediated biotransformations – Bio-catalyst mediated Baeyer-Villiger reactions – Microbial polyester synthesis.



### **UNIT -V: Alternative Synthesis, Reagents and Reaction Conditions**

A photochemical alternative to Friedel-crafts reactions - Dimethyl carbonate as a methylating agent – the design and applications of green oxidants – super critical carbon dioxide for synthetic chemistry.

#### **Text Book**

1. RashmiSanghi&M. M. Srivastava, Green Chemistry – Environment friendly alternatives, Narora Publishing House, 2003.

#### **Reference Books**

1. V. K. Ahluwalia, Green Chemistry – Environmentally benign reactions, Ane Books India, 2006.
2. Green Chemistry – Designing Chemistry for the Environment – edited byPaul T. Anastas& Tracy C. Williamson. Second Edition, 1998.
3. Green Chemistry – Frontiers in benign chemical synthesis and processes- edited byPaul T. Anastas& Tracy C. Williamson. Oxford University Press, 1998.

**SEMESTER-III: CORE COURSE-X: PHYSICAL CHEMISTRY-II**

**Course Code :P3RCHCC10**

**Max. Marks : 100**

**Hours/Week : 5**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To understand the electro chemistry*
- ❖ *To know Molecular Thermodynamics*
- ❖ *To understand the surface phenomena*
- ❖ *To understand quantum chemistry and their application to spectroscopy*

**UNIT – I: Electrochemistry-I**

Electrolytic conductance Debye-Huckel-Onsager theory – Debye Falkenhagen and Wien effect. Electrode – electrolyte equilibrium, electrode potential – concentration cells – liquid junction potentials. Processes at Electrodes- The rate of charge transfer - current density – Butler – Volmer Equation – Tafel equation – Electrical double layer potential – Theory of multiple layers at electrode – electrolyte interfaces – Double layer capacity – Electrokinetic phenomena, Applications: Fuel cells and power storage.

**UNIT – II: Electrochemistry-II**

Principles and applications of polarography – Instrumentation, Types of cells, advantages of dropping mercury electrode, interpretation of current voltage curves, tests for reversibility, determination of 'n' values (usefulness of Ilkovic equation), polarographic maxima, current time curves, Modern developments, Oscillographic polarography, AC polarography – Cyclic Voltammetry, advantages over polarographic techniques – test of reversibility of electron transfer reactions – Chronopotentiometry – apparatus used, advantages over polarography – controlled potential coulometry.

**UNIT – III: Molecular Thermodynamics-II**

Third law-thermodynamics-Need for it-Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities at absolute zero – Apparent exceptions to the third law. Thermodynamics of systems of variable composition – partial molar properties – chemical potential – relationship between partial molar quantities – Gibbs Duhem equation and its applications (the experimental determination of partial molar properties not included). Thermodynamic properties of real gases – fugacity concept – calculation of fugacity of

real gas–Activity and activity coefficient – concept – definition – standard states and experimental determinations of activity and activity coefficient of electrolytes.

#### **UNIT – IV: Surface Phenomena**

Surface Phenomena: Gibbs adsorption isotherm–solid- liquid interfaces–contact angle and wetting–solid-gas interface–physisorption and chemisorptions–Langmuir, BET isotherms–surface area determination. Kinetics of surface reactions involving adsorbed species–Langmuir-Hinshelwood mechanism, Langmuir–Rideal mechanism-Rideal–Eley mechanism. Some interfacial aspects on Micelles, Reverse micelles, Micro emulsions and Membranes.

#### **UNIT – V: Quantum Chemistry**

Applications of Wave mechanics, the rigid rotator, harmonic oscillator – Hydrogen atom solution – Shapes and nodal properties of orbitals – Space quantisation – electron spin – Many electron atoms – one electron orbitals – Pauli principle – determine form of wave function, Helium atom and effective nuclear charge- Approximation methods – Variation methods, application to Hydrogen and Helium atoms–Perturbation method for nondegenerate systems. Angular momentum in many electron systems – Spin orbit interaction, L-S and j-j coupling schemes. Atomic Structure Calculation – Self consistent field method for atoms – Hartree and Hartree Fock method for atoms. Vibrational spectra – symmetry properties of normal molecules – Symmetry co-ordinates – Selection rules for fundamental vibrational transition – IR and Raman activity of fundamentals in CO<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>F<sub>2</sub> – The rule of mutual exclusion and fermi resonance.

#### **Text Book**

1. F.A. Cotton, Chemical Applications of group Theory, 2<sup>nd</sup> Ed., Wiley Eastern 1971
2. A.K. Chandra, Introductory Quantum Chemistry, 4<sup>th</sup> Ed., Tata McGraw Hill, 1994
3. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1983.
4. J.P. Lowe, Quantum Chemistry, Academic Press, 1978.
5. I.N. Levine, Quantum Chemistry, Allyn and Bacon, 1983.
6. S.Glasstone, Introduction to Electrochemistry, Affiliated East-West Press, 1968.
7. J.Albery, Electrode Kinetics, Clarendon Press, Oxford Chemical Series, 1979.

**References Books:**

1. P.W. Atkins, Physical Chemistry, ELBS and Oxford University Press, Oxford, 1983.
2. D.R.Crow, Polarography of Metal Complexes, Academic Press, New York.
3. Daniel C Harris, Quantitative Chemical Analysis, 4<sup>th</sup> ed., W. H. Freeman and Company, New York, **1995**
4. J. Rajaram and J.C.Kuriacose, Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, Shobhan Lal Nagin, New Delhi, **1981**.
5. G.W.Castellan, Physical Chemistry, Narosa, New Delhi, **1986**.
6. M. Klotz and P.M.Rosenberg, Chemical Thermodynamics: Basic Theory and Methods, 3 Edn. W.A.Benjamin, New York, **1974**.
7. K.J. Laidler, Chemical Kinetics, 2<sup>nd</sup> Ed., Tata McGraw Hill, **1975**.

**SEMESTER-III: CORE COURSE-XI: INORGANIC CHEMISTRY-II**

**Course Code :P3RCHCC11**

**Max. Marks : 100**

**Hours/Week : 5**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To understand the principal of bioorganic chemistry*
- ❖ *To know the cobalamine and Heme protein*
- ❖ *To understand the medicinal bioorganic chemistry*
- ❖ *To understand the metallocene and organometallic reaction*

**UNIT – I: General Principles of Bioinorganic Chemistry**

Occurrence and availability of Inorganic elements in biological systems. **Biomineralisation** Control and assembly of advanced materials in Biology - Nucleation and crystal growth – various biominerals – calcium phosphate – calcium carbonate – Amorphous silica, Iron biominerals – strontium and barium sulphate. **Function and Transport of Alkali and Alkaline Earth Metal Ions:** Characterization of  $K^+$ ,  $Na^+$ ,  $Ca^{2+}$  and  $Mg^{2+}$  - complexes of alkali and alkaline earth metal ions with macrocycles - Ion channels – ion pumps. Catalysis and regulation of bioenergetics processes by the Alkaline Earth Metal ions  $Mg^{2+}$  and  $Ca^{2+}$ . **Metals at the Center of Photosynthesis:** Primary Processes in Photosynthesis – Photosystems I and II - Light Absorption (Energy Acquisition) – Exciton transport (Direct Energy Transfer) – Charge separation and electron transport – Manganese catalyzed oxidation of water to  $O_2$ .

**UNIT – II**

**Cobalamines** Reactions of the alkyl cobalamins – One-electron Reduction and Oxidation – Co-C Bond Cleavage – coenzyme B12 – Alkylation reactions of methylcobalamin. **Heme and Non-heme Proteins** Hemoglobin and Myoglobin – Oxygen transport and storage – Electron transfer and Oxygen activation. Cytochromes, Ferredoxins and Rubredoxins – Model systems, mononuclear non-heme iron enzymes. **Copper Containing Proteins** Classification and examples - Electron transfer – Oxygen transport - Oxygenation – oxidases and reductases – Cytochrome c oxidase – Superoxide dismutase (Cu, Zn). **Nickel containing Enzyme:** Urease.

### UNIT – III

**Medicinal Bioinorganic Chemistry:** Bioinorganic Chemistry of quint essentially toxic metals. Lead, Cadmium, Mercury, Aluminum, Chromium, Iron, Copper, Plutonium. Detoxification by metal chelation. Drugs that act by binding at the metal sites of Metalloenzymes. **Chemotherapy** Chemotherapy with compounds of certain non-essential elements. Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action - Lithium in Psychopharmacological drugs. Radiopharmaceuticals – Technetium.

### UNIT IV

Hapticity, Ligand classification, synthesis and structure – The 18 electron rule – application and limitation-isolobal concept and its usefulness. Uses of typical organometallics in organic synthesis such as metal alloys and organometallic hydrides. Structure and bonding in metal carbonyls (simple and polynuclear) nitrosyl complexes – bridging and terminal nitrosyls, bent and linear nitrosyls. Dinitrogen complexes. Metallocene and arene complexes. Metal carbenes, carbynes, carboxylate anions.

### UNIT – V

**Reactions and Catalysis by Organometallics:** Organometallic reactions – Ligand association and dissociation – oxidative addition and reductive elimination – Insertion reactions – Reactions of coordinated ligands in organometallics- Hydrogenation, hydroformylation, epoxidation, metathesis, polymerization of olefins, olefin oxidation (Wacker process) and carbonylation of methanol.

#### Text Books and Reference Books

1. J. E. Huheey, Inorganic Chemistry, 3<sup>rd</sup> Ed., Harper & Row Publishers, Singapore.
2. Purcell and Kotz, Inorganic Chemistry, Saunders Golden Sunburst Series, W. B. Saunders Company, Philadelphia.
3. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, 1997.
4. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA.

5. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup>Ed., Wiley IntersciencePublication, John Wiley & Sons, New York, USA.
6. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley & Sons, NewYork.
7. B. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic
8. Chemistry, 2<sup>nd</sup> Ed, John Wiley & sons, New York.
9. J. P. Collman, L. S. Hegedus, J. R. Nortan and R. G. Finke, Principles and Applications ofOrganotransition Metal Chemistry, University Science Books. Mill Valley, California.

**SEMESTER-III: CORE COURSE-XII: PHYSICAL METHODS IN CHEMISTRY – II**

**Course Code :P3RCHCC12**

**Max. Marks : 100**

**Hours/Week : 5**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To understand the principles of electronic and vibrational spectroscopy and their applications*
- ❖ *To understand the principles of NMR, EPR and Mossbauer Spectroscopy and their application*

**UNIT-I: 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 parameter B and C. R-S coupling and jj coupling. selection rule and breakdown of selection rules-Group theoretical explanation. Ground states of free ion for  $d^n$  system-octahedral and tetrahedral system and the corresponding energy level diagrams-mixing of orbitals. Orgal diagram-characteristics-prediction and assignment of transition for  $d^n$  weak field cases. Tanane-sugano diagrams-characteristics- prediction and assignment of transition for weak field and strong field  $d^n$  systems, band widths-band shape, band intensity-Effect of distortion and spin-orbit coupling on spectra – Evaluation of  $10Dq$  and B for octahedral complexes of cobalt and nickel – charge transfer spectra

**UNIT – II: Infrared and Raman Spectroscopy**

Vibrations in simple molecules ( $H_2O, CO_2$ ) and their symmetry notation for molecular vibrations – Group vibrations and the limitations- combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like  $N_2O, ClF_3, NO_3^-, ClO_4^-$  –effect of coordination on ligand vibrations–uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide–Effect of isotopic substitution on the vibrational spectra of molecules–vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment)–Applications of Raman Spectroscopy–Resonance Raman Spectroscopy. Mass Spectrometry: Principles and presentation of spectra–molecular fragmentation–ion reactions–Inorganic applications.



### **UNIT-III: NMR Spectroscopy**

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei ( $^1\text{H}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{13}\text{C}$ ) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei ( $^2\text{H}$ ,  $^{10}\text{B}$ ,  $^{11}\text{B}$ ) on the  $^1\text{H}$  NMR spectra, Satellite spectra. Systems with chemical exchange - evaluation of thermodynamic parameters in simple systems – study of fluxional behavior of molecules – an elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents.

### **UNIT-IV: EPR spectroscopy**

Theory of EPR spectroscopy-Spin densities and McConnell relationship-Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy-Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions. **Magnetic properties:** Types of magnetism-Dia-para-ferro and anti-ferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Second order Zeeman effect – states  $KT$  – states  $\ll KT$ . Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism. Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds.

### **UNIT-V: Mossbauer Spectroscopy**

Isomer shifts-Magnetic interactions-Mossbauer emission spectroscopy-applications to iron and tin compounds. **NQR spectroscopy:** Characteristics of quadrupolar nucleus-effects of field gradient and magnetic field upon quadrupole energy levels-NQR transitions-applications of NQR spectroscopy.

#### **Text Books**

1. R.S. Drago, Physical Methods in Inorganic Chemistry, 3<sup>rd</sup> Ed., Wiley Eastern Company.
2. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders Company, Philadelphia, London.
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 3<sup>rd</sup> Ed., Wiley-Eastern Company, New Delhi, 1990.
4. E.A.V. Ebsworth, Structural Methods in Inorganic Chemistry, 3<sup>rd</sup> Ed., ELBS, Great Britain, 1987.

**SEMESTER-III: ELECTIVE COURSE-III: SUPRAMOLECULAR CHEMISTRY &  
CRYSTAL ENGINEERING**

**Course Code :P3RCHEC3**

**Hours/Week : 5**

**Credit : 3**

**Max. Marks : 100**

**Internal Marks : 25**

**External Marks : 75**

**Objectives**

- ❖ *To understand the supramolecular chemistry*
- ❖ *To understand the metallo organic frame works and nano porous materials and their applications.*
- ❖ *To understand the application of supramolecular chemistry to catalysis, devices and sensors*

**UNIT-I: Concepts and Languages of supramolecular chemistry**

Concepts and Languages of supramolecular chemistry. Various types of non-covalent interactions. Hydrogen bonds, C-H...X interactions, Halogen bonds.  $\pi - \pi$  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 Frame works**

M.O.F (Metallo Organic Frame works), Organometallic systems. Combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. Design of nanoporous solids. Inter ligand hydrogen bonds in metal complexes – implications for drug design. Crystal engineering of NLO materials, OLED.

**UNIT-III: Coreceptor Molecules and Multiple Recognition**

Coreceptor Molecules and Multiple Recognition: Dinuclear and Polynuclear Metal ion Cryptates. Linear recognition of molecular length by Ditungstic Coreceptors. Heterotopic Coreceptors- Cyclophane Receptors, Amphiphilic Receptors, Large molecular cages. Multiple Recognition in Metallo receptors. Supramolecular dynamics.

#### **UNIT-IV: Supramolecular Reactivity and Catalysis**

Supramolecular Reactivity and Catalysis: Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules. Catalysis with Cyclophane Type Receptors. Supramolecular Metallo catalysis. 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 and Sensors**

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: Photo switching and Electroswitching. Ion and molecule sensors. Role of supramolecular chemistry in the development of nano-science and technology.

#### **References Books:**

1. Lehn, J.M. Supramolecular Chemistry, VCH, Weinheim, 1995.
2. Desiraju, G.R. Crystal Engineering: The Design of Organic Solids, Elsevier, Amsterdam, 1989.
3. Desiraju, G.R. & Steiner, T. The weak Hydrogen Bond in Structural Chemistry and Biology: Oxford University press: Oxford, 1999
4. Anthony R. West, Solid state chemistry and its applications by, John Wiley & sons

**SEMESTER-III: CORE COURSE-XIII:PHYSICAL CHEMISTRY PRACTICAL-I**

**Course Code :P3RCHCC13P**

**Max. Marks : 100**

**Hours/Week : 6**

**Internal Marks : 40**

**Credit : 5**

**External Marks : 60**

**Objective**

- ❖ *To learn some non-electrical physical chemistry experiments*
- ❖ *To study the kinetics of some reactions and phase diagram of some binary system*
- ❖ *To learn the determination methods of physical constants of substances*

Any ten experiments out of the following experiments.

1. Kinetics- Acid hydrolysis of Ester- Comparison of strengths of acids.
2. Kinetics- acid hydrolysis of Ester- Determination of energy of activation (Ea).
3. Kinetics- Saponification of Ester- Determination of Ea by conductometry.
4. Kinetics- Persulphate- Iodine reaction- Determination of order, effective of ionic strength on rateconstant.
5. Determination of molecular weight of substance by Transition Temperature method.
6. Determination of molecular weight of substances by Rast method.
7. Determination of Critical Solution Temperature (CST) of phenol- water system and effect of impurity on CST.
8. Study of phase diagram of two components forming a simple eutectic.
9. Study of phase diagram of two compounds forming a compound.
10. Study of phase diagram of three components system.
11. Determination of molecular weight of substances by cryoscopy.
12. Determination of integral and differential heat of solutions by colorimetry.
13. Polymerization- Rate of polymerization of acrylamide.
14. Distribution law- Study of Iodine- Iodine equilibrium.
15. Distribution law- Study of association of benzoic acid in benzene.
16. Adsorption- Oxalic acid/Acetic acid on charcoal using freundlich isotherm.

**Reference books**

1. J.B.Yadav, “ Advanced Practical Physical chemistry”, 20<sup>th</sup> Ed., GOEL publishing House, KrishnaPakashan Media Ltd., (2001).
2. Findlay’s “Practical Physical Chemistry” Revised and edited by B.P. Levitt 9th ed., Longman,London, 1985.
3. J.N. Gurtur and R.Kapoor, “Advanced Experimental chemistry”, Vol.I. Chand & Co., Ltd, New Delhi.

**SEMESTER-III: CORE COURSE-I:PHYSICAL CHEMISTRY PRACTICAL-II**

**Course Code :P3RCHCC14P**

**Max. Marks : 100**

**Hours/Week : 6**

**Internal Marks : 40**

**Credit : 5**

**External Marks : 60**

**Objectives**

- ❖ *To learn some electro analytical experiments*

Any ten experiments out of the following experiments.

- a. Conductometry- Acid- alkali titrations.
- b. Cuctometry- Precipitation titrations.
- c. Conductometry- Displacement titrations.
- d. Conductometry- Determination of dissociation constant of weak acids.
- e. Conductometry- solubility product of sparingly soluble silver salts.
- f. Verification of Onsager equation- conductivity method.
- g. Determination of degree of hydrolysis and hydrolysis constant of a substance.
- h. Potentiometric titrations- Acid alkali titrations.
- i. Potentiometric titrations- Precipitation titrations.
- j. Potentiometric titrations- Redox titrations.
- k. Potentiometry- Determination of dissociation constant of weak acids.
- l. Potentiometry- Determination of solubility of silver salts.
- m. Potentiometry- Determination of activity and activity coefficient of ions.
- n. *pH*titration of *ortho*-phosphoric acid.
- o. To determine the relative strength of two acids by conductance measurements.
- p. To determine the pH of a buffer solution using a quinhydrone electrode.

**Reference books**

1. J.B.Yadav, "Advanced Practical Physical chemistry", 20<sup>th</sup> Ed., GOEL publishing House, KrishnaPakashan Media Ltd., (2001).
2. Findlay's "Practical Physical Chemistry" Revised and edited by B.P. Levitt 9th ed., Longman,London, 1985.
3. J.N. Gurtur and R.Kapoor, "Advanced Experimental chemistry", Vol.I. Chand & Co., Ltd, New Delhi.

**SEMESTER-III: ELECTIVE COURSE-III: NATURAL PRODUCTS**

**Course Code :P3RCHEC3**

**Hours/Week : 5**

**Credit : 3**

**Max. Marks : 100**

**Internal Marks : 25**

**External Marks : 75**

**Objectives**

- ❖ *To understand the some important natural pigments and terpenoids*
- ❖ *To understand the biosynthesis of natural products and steroids*

**UNIT-1: Natural pigments I**

Introduction to Natural pigments, Classification of pigments, **Carotenoids**-Introduction-Classification-Isolation and Separation of carotenoids-Characteristics-function-elucidation of constitution-synthesis. **Anthocyanins**-Introduction-Classification-Isolation-Functions-Synthesis-Elucidation of constitution. **Flavones**-Introduction-properties –Isolation-Separation and purification-Elucidation of structure-synthesis. **Flavonols**-Introduction-Elucidation of structure-Synthesis. **Isoflavones**-Introduction-Distinction of Isoflavones from flavones and isoflavonones-Determination of structure of isoflavones. **Xanthones**-Introduction-preparation-properties-synthesis.

**UNIT-II: Alkaloids**

Alkaloids: Definition, occurrence, extraction of alkaloids from plants, general properties, determination of the chemical constitution of the alkaloids, functional group analysis, estimation of groups, degradation and synthesis. Preparation, properties and structural elucidation of Coniine, Piperine, nicotine and ephedrine.

**UNIT-III: Terpenoids**

Introduction-Nomenclature-properties-Isolation-Isoprene rule-Gem-dialkyl rule-Determination of structures of terpenoids. **Myrcene**-Introduction-Elucidation of constitution-Synthesis. **Citral**-Introduction-Isolation-Elucidation of constitution-Synthesis. **Menthone**-Introduction-Elucidation of constitution-Synthesis. **Irones**- Introduction-Elucidation of constitution-Synthesis. **Carone**-Introduction-Elucidation of constitution-Synthesis.

**UNIT-IV: Bio Synthesis of Some Natural Products**

Introduction, Bio synthesis of Terpenoids, Steroids, Oestrogens, Gestrogens, Corticoids and Alkaloids.

### **UNIT-V: Steroids**

Cholesterol-Introduction-Elucidation of constitution. **Stigmasterol**-Introduction-Elucidation of constitution. **Ergosterol**-Introduction-Elucidation of constitution. Sex hormones-Introduction-**Oestrogen**- Oestrone- Introduction-Elucidation of constitution.**Progesterone**- Introduction-Elucidation of constitution.**Androsterone**- Introduction-Elucidation of constitution.

### **Reference Book**

1. I. L. Finar, Organic Chemistry, Vol I & II, 6<sup>th</sup> Ed., England, Wesley Longman Ltd. (1996).
2. Gurdeep Chatwal and Anand, Chemistry of Natural Products, Himalayan Publishing Co, 2001.
3. O. P. Agarwal, Chemistry of Natural Products, Vol-1, 2, Goel Publishing House, 1997.

**SEMESTER-IV: ELECTIVE COURSE-I:ADVANCED TOPICS IN CHEMISTRY**

**Course Code :P4RCHEC4**

**Hours/Week : 6**

**Credit : 5**

**Max. Marks : 100**

**Internal Marks : 25**

**External Marks : 75**

**Objectives**

- ❖ *To understand the concepts of supramolecular chemistry and various non-bonded interactions*
- ❖ *To understand the principle of solid state chemistry and electro organic synthesis*
- ❖ *To understand the nano-materials and synthetic methods and their characterization techniques*

**UNIT-1: Concepts of Supramolecular Chemistry**

Concepts and Languages of supramolecular chemistry. Various types of non-covalent interactions. Hydrogen bonds, C-H...X interactions, Halogen bonds.  $\pi - \pi$  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: Preparative methods in solid state chemistry**

General principles of solid state chemistry-Experimental procedure, Co-precipitation 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, Melts, Glasses - Vapour phase transport methods - Modification of existing structures by ion exchange and intercalation reactions, 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 and Stockbarger methods, Zone melting, Precipitation from solution or melt: flux method, Epitaxial growth of thin layers, Verneuil flame fusion method, Vapour phase transfer, Hydrothermal methods, Comparison of different methods - High pressure and hydrothermal methods, Hydrothermal methods, Dry high pressure methods.



### **UNIT-III: Basic concepts of electro organic synthesis**

Introduction, fundamental aspects of electro transfer reaction: oxidation, reduction reactions vs electrontransfer reactions in organic chemistry and electrochemistry - Standard potentials: Mechanism and theoryof outer sphere electron transfer reactions – Fundamental aspects of electrode phenomena, monitoring a half-reactions, general view of an electrode reaction, adsorption phenomena – Mass transfer in electrochemistry, fundamental aspects, steady state electrochemical methods, Transient electrochemicalmethods.

### **UNIT-IV: Nanomaterials – An Introduction & Synthetic methods**

Definition of nanodimensional materials - Historical milestones - unique properties due tonanosize, Quantum dots, Classification of Nanomaterials. General methods of synthesis of nanomaterials –Hydrothermal synthesis, Solvothermal synthesis, Microwave irradiation, sol – gel and Precipitation technologies, Combustion Flame-Chemical Vapor Condensation Process, gas Phase Condensation Synthesis, Reverse Micelle Synthesis, Polymer – Mediated Synthesis, Protein Microtube – Mediated Synthesis, Synthesis of Nanomaterials using microorganisms and other biological agents, Sonochemical Synthesis, Hydrodynamic Cavitation. Inorganic nanomaterials – Typical examples – nano TiO<sub>2</sub> / ZnO/CdO/CdS, Organic nanomaterials – examples – Rotaxanes and Catenanes.

### **UNIT-V: Techniques for Characterization of nanoscale materials**

Principles of Atomic force microscopy (AFM)-Transmission electron microscopy (TEM)- Resolution and scanning transition electron microscopy (STEM) Scanning Tunneling Microscopy (STM) Scanning nearfield optical microscopy (SNOM), Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasma on spectroscopy.

#### **Reference Books:**

1. Solid state chemistry and its applications by Anthony R. West, John Wiley & sons
2. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
3. Desiraju, G.R. Crystal Engineering: The Design of Organic Solids, Elsevier, Amsterdam, 1989.

#### **Journals:**

1. Crystal Growth and Design, <http://www.pubs.acs.org/journals/cgdefu/index.html>
2. Crystal Engineering Communication, <http://www.rsc.org/Publishing/Journals/ce/index.asp>
3. Nano letters - <http://pubs.acs.org/journals/nalefd/index.html>

**SEMESTER-IV: ELECTIVE COURSE-IV:ANALYTICAL CHEMISTRY**

**Course Code :P4RCHEC4**

**Max. Marks : 100**

**Hours/Week : 6**

**Internal Marks : 25**

**Credit : 5**

**External Marks : 75**

**Objectives**

- ❖ *To understand the Instrumental methods of various spectroscopy*
- ❖ *To acquire skill of calculation of analytical data*
- ❖ *To understand the electroanalytical techniques and thermo analytical methods in analytical techniques*

**UNIT-I: 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: Data and Error Analysis**

Various types of Error–Accuracy, precision, significant figures–Frequency distributions, the binomial distribution, the Poisson distribution and normal distribution–Describing data, population and sample, mean, variance, standard deviation, way of quoting uncertainty, robust estimators, repeatability and reproducibility of measurements–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: 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: Thermo Analytical Methods**

Principles, factors affecting thermogram, instrumentation and thermal decomposition of  $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$  and  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ . Differential technique: Instrumentation, experimental, instrumental factors of DTA and DSC. Thermal studies of  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  by DTA and determination of purity of pharmaceuticals and phase transition studies by DSC – evaluation and thermodynamic parameters. Electrogravimetry: Principle, instrumentation, deposition and separation. Electrolysis at constant. Thermometric titrations.

#### **UNIT-V: Electroanalytical Techniques and Fluorescence Spectroscopy**

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 – Amperometric gas sensors – Amperometric titrations: Principles- Apparatus – techniques – applications. Basic aspects of synchronous fluorescence spectroscopy – Spectral hole burning – flow cytometry – Instrumentation on fluorescence ratio – Fluorimeters (quantization).

#### **References Books**

1. Analysis for chemistry, Oxford University Press, 2006.
2. J. Topping, Errors of Observation and their treatment, 4<sup>th</sup> Ed., Chapman Hall, London, 1984.
3. R. Stock and C. B. F. Rice, Chromatographic Methods, Chapman and Hall, New York.
4. V.K. Srivastava and K.K. Srivastava, Introduction to Chromatography, S. Chand & Co., New Delhi, 2<sup>nd</sup> Ed, 1981.
5. Willard, Merrit, Dean and Settle, Instrumental methods of Analysis CBS Publishers and Distributors, 6<sup>th</sup> Ed., 1986.
6. D. A. Skoog, D.M. West, F.J. Holler, F. J., Fundamentals of Analytical Chemistry, 7<sup>th</sup> Ed., Harcourt College Publishers, Singapore.
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<sup>th</sup> Ed., Tata McGraw-Hill, New Delhi, 1994.
9. Vogel, A. I., Text book of Quantitative Inorganic Analysis, ELBS.
10. Daniel C Harris, Quantitative Chemical Analysis, 4<sup>th</sup> Ed., W. H. Freeman and Company, New York, 1995.
11. S.C. Gupta, Fundamentals of Statistics, 6<sup>th</sup> Ed., Himalaya Publ. House, Delhi, 2006.