Post - Graduate Programme in Chemistry

Courses of study, Schemes of Examinations & Syllabi

(Choice Based Credit System)

DEPARTMENT OF CHEMISTRY
(DST – FIST sponsored)
BISHOP HEBER COLLEGE (Autonomous)
(Reaccredited with 'A' Grade (CGPA – 3.58/4.0) by the NAAC &
Identified as College of Excellence by the UGC)
DST – FIST Sponsored College &
DBT Star College
TIRUCHIRAPPALLI – 620 017
TAMIL NADU, INDIA

2017

Post – Graduate Programme in Chemistry

Structure of the Curriculum

Parts of the Curriculum	**No. of courses**	**Credits**
Core Course (theory)	9	50
Core Course (practical)	6	18
Elective	4	14
Project	1	4
NMEC	1	2
VLOC	1	2
Total	**22**	**90**

M.Sc., Chemistry
(For the candidates admitted from the academic year 2016 onwards)

Sem.	Course	Course Code	Course Title	Pre requisites	Hrs./ week	Credits	Marks		
							CIA	ESA	Total
I	Core I	P16CH101	Inorganic Chemistry- I		6	6	25	75	100
	Core II	P16CH102	Basic Concepts in Organic Chemistry		6	6	25	75	100
	Core III	P16CH103	Physical Chemistry -I		6	6	25	75	100
	Core Prac. I	P16CH1P1	Inorganic Chemistry Practical - I		6	3	40	60	100
	Core Prac. II	P16CH1P2	Organic Chemistry Practical - I		6	3	40	60	100
II	Core IV	P16CH204	Inorganic Chemistry- II		6	6	25	75	100
	Core V	P16CH205	Reactions and Mechanisms in Organic Chemistry	P16CH102	6	6	25	75	100
	Core Prac. III	P16CH2P3	Inorganic Chemistry Practical - II		6	3	40	60	100
	Core Prac. IV	P16CH2P4	Organic Chemistry Practical - II		6	3	40	60	100
	NMEC		***To be selected from the courses offered by other departments***		4	2	25/ 40	75/ 60	100
	VLOC	P17VL2:1/ P17VL2:2	RI / MI		2	2	25	75	100
III	Core VI	P16CH306	Organic Spectroscopy		6	5	25	75	100
	Core VII	P16CH307	Physical Chemistry -II		6	5	25	75	100
	Core Prac. V	P16CH3P5	Physical Chemistry Practical - I	P16CH103	6	3	40	60	100
	Core Prac. VI	P16CH3P6	Physical Chemistry Practical - II	P16CH103	6	3	40	60	100
	Elective I	P16CH3:1/ P16CH3:2	Analytical Techniques and C Programming / Green Chemistry		5	4	25	75	100
	Project	P16CH4PJ	Project		1	-			
IV	Core VIII	P16CH408	Inorganic Chemistry-III		6	5	25	75	100
	Core IX	P16CH409	Physical Chemistry - III		6	5	25	75	100
	Elective II	P16CH4:2	Principles and application of Drug design and Discovery	P16CH102 P16CH205	5	4	25	75	100
	Elective III	P16CH4:3	Bio-Inorganic Chemistry		5	4	25	75	100
	Elective IV	P16CH4:P	Computational Chemistry and Drug Designing - Practical	P16CH102, P16CH4:2	3	2	40	60	100
	Core Project	P16CH4PJ	Project		5	4	--	--	100
Total						**90**			**2200**

CIA- Continuous Internal Assessment
ESA- End Semester Assessment
NMEC- Non Major Elective Course
VLOC- Value added Life Oriented Course

List of Elective Courses:

1. Green Chemistry
2. Analytical Techniques in Chemistry
3. Radiation Chemistry
4. Natural Products Chemistry
5. Chemistryof Polymers

NMEC offered to students of other departments:

1. Chemistryfor Healthy Living

CORE COURSE I : INORGANIC CHEMISTRY – I

Semester: I **Code : P16CH101**
Credits : 6 **Total Hrs: 90**

General Objectives

1. To understand the trends in periodic properties and acid-base concepts.
2. To identify the nature of chemical bond in a given inorganic compound.
3. To learn the basic concepts of nuclear chemistry.
4. To know nuclear and radioisotopes techniques.
5. To understand the appropriate importance of catenation and heterocatenation
6. To identify iso and heteropoly anions for specific applications.

UNIT-I

1 .1 Acids and Bases

Differentiating and levelling solvents - Usanovich and Lux Flood concepts - Solvent ion theory of acids and bases -Hard and Soft Acids and Bases (HSAB)- Classification, acid-base strength and hardness and softness - Symbiosis - Theories of hardness and softness - Electronegativity and hardness and softness - Applications of HSAB, proton sponges

1.2 Non aqueous solvents: Classification - protic and aprotic solvents, – Liquid NH_3, BrF_3, CH_3COOH, liquid SO_2, liquid HF. (Proton sponges- molten salts as solvents and ionic liquids)

UNIT–II Ionic Bonding and Crystal Structure

2.1 Packing of ions in crystals & crystal structure - ccp, hcp, bcc, fcc

2.2 Radius ratio and structure of ionic lattices, Calculation of radius ratio and Coordination No, stoichiometry and crystal structures of NaCl, CsCl, Zincblende, Wurtzite, Rutile, Flourite, Antifluorite, Perovskite, CdI_2, β- cristobalite & ReO_3 structure, Spinels and Inverse Spinels.

2.3 Lattice energy- Slater's rule, Born-Haber cycle - Born-Lande equation, Factors affecting Lattice Energy

2.4 Crystal defects: Stoichiometric and non stoichiometric defects. Metal excess defects - Metal deficiency defects - calculation of number of defects.

UNIT-III

3.1 Nuclear Chemistry

Nucleus- Structure of the nucleus, Radioactive equilibrium, Orbital electron capture, Nuclear isomerism, Internal conversion, Nuclear cross section.

Nuclear stability- Binding energy, shell model, magic numbers, Harkin's rule, Theories of decay processes - Geiger-Nuttal rule, Group displacement laws and units of radioactivity

3.2 Radioactivity

Nuclear reactions: Q- value of nuclear reactions, transmutation, stripping and pickup, fission, fusion, spallation, projectile capture and particle emission reaction, fragmentation and scattering.

Particle accelerators: Cyclotron, linear accelerator and synchrotron

Nuclear reactors: Power reactor, breeder and Fast breeder reactors

Radioactive techniques: Tracer technique, Neutron activation and Isotopic dilution analysis.

Counting techniques: Geiger-.Muller, scintillation and proportional counters.

Applications: Carbon dating, agriculture, medicine and industry.

UNIT-IV Covalent Bonding

4.1 VBT: Resonance, conditions for resonance, formal charges, hybridization and geometry, VSEPR model- CH_4, NH_3, H_2O, PCl_3,F_2- Bents' rule- SF_4, BrF_3, ICl_2^-, ICl_4^-, XeF_4, $XeOF_4$, XeO_4, XeO_3, XeF_6, XeF_2

4.2 MOT: LCAO method - MO level energy level diagram of hetero diatomic molecule (HCl) and polyatomic molecule NH_3 and SF_6 - LUMO and HOMO concepts in bonding.

4.3 Bonding in metals: Band theory of solids, Insulators, Semiconductors n and p type, Super conductors and its applications.

UNIT-V Inorganic Chain , Ring & Cage Compounds

5.1 Electron deficient , electron precise and electron rich compounds: **Boranes and Carboranes**: Structure of B_2H_6 , B_4H_{10}, B_{12} H_{12}^{2-} ,B_6 H_{10}, B_8H_{12}, $B_{10}H_{14}$. Synthesis of neutral boron hydrides, polyhedral boron anions and dianions, structure of polyhedral boranes-nido-arachno - and closo-frameworks, PSEPT (wade's rule and styx code). Carboranes-synthesis, polyhedral geometries of metalloboranes and metallocarboranes.

5.2 Boron –Nitrogen compounds: Structure and bonding of $B_3N_3H_6$, Borazines, B-N clusters and azaboranes.

5.3 Metal clusters: Structure and bonding of dinuclear cluster $Re_2Cl_8^{2-}$

5.4 Poly acids: Structure of isopoly and heteropoly anions and polycations of W and Mo.

5.5 P-N and P-S compounds: Polyphosphazene, cyclophosphazene, P-S cages.

5.6 Cyclic S-N compounds: Tetra sulphur - tetranitride (S_4N_4) and Polythiazyl.

Recommended Books

1. Bodie E. Douglas and Darl H. Mc Daniel, John J. Alexander, *Concepts and Models in Inorganic Chemistry*, Wiley Eastern, New Delhi, 2006.
2. J.D. Lee, A New Concise Inorganic Chemistry, ELBS, New Delhi, 1995.
3. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, Saunders Golden Sunburst Series, E.B. Saunders Company, Philadelphia, 1977.
4. F.Albert Cotton, Geoffrey Wilkinson and Carlos A. Murillo, Advanced Inorganic Chemistry, John Wiley and Sons, Singapore, 2003.
5. B.R. Puri, L.R. Sharma and K.C. Kalia ,Principles of Inorganic Chemistry - Vishal Publishing Co., Jalandhar, 2007.
6. S. Glasstone, Source book on Atomic Energy- 3rd edition, Affiliated East-West Press Pvt. Ltd., New Delhi, 1967.
7. Alan G. Sharp, Inorganic Chemistry, Addison - Wesley, New York, 1999.
8. Gary L. Miessler, Donald A. Tarr, Inorganic Chemistry, Pearson Education, New Delhi,2004.
9. James E. Huheey, Ellen A Keiter and Richard L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, Addison-Wesley, New York, 2003. **(Unit- I, II, IV, V)**
10. H.J. Arnikar, Essentials of Nuclear Chemistry, New Age International, New Delhi,1995. **(Unit- III)**

CORE COURSE II : BASIC CONCEPTS IN ORGANIC CHEMISTRY

Semester: I **Code : P16CH102**
Credits : 6 **Total Hrs: 90**

General Objectives

1. To understand the basic concepts of aromaticity
2. To name organic compounds by IUPAC rules
3. To comprehend the various factors that operate in organic reactions
4. To appreciate the stereochemical aspects of a reaction

UNIT– I Nomenclature of Organic Compounds

1.1 Nomenclature - General rules - Naming of linear and branched alkanes, alkenes, polyenes and alkynes with two or three functional groups by IUPAC nomenclature. Aromatic and heteroaromatic systems - nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Fused heterocycles and fused aromatic systems.

1.2 Nomenclature of alicyclic, bicyclic and tricyclic compounds - organic molecules including regio and stereoisomers.

UNIT–II Reaction Mechanisms and Intermediates

2.1 Reaction Mechanism: Structure and Reactivity

Types of reactions, Types of mechanisms , Rate constants - determination and life times of reactive energy states - Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Quantitative treatment. The Hammett equation and I inear free energy relationship, substituent and reaction constants. Taft equation.

2.2 Reactive Intermediates

Free radicals, carbenes, nitrenes, carbanions, classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations.

UNIT–III Aromaticity of Organic Compounds

3.1 Aromaticity

Electron delocalization and resonance - Huckel's rule - Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons - Craigs rule (fused ring system)- Aromaticity on larger annulenes - antiaromatic - homoaromatic and non-aromatic compounds -Molecular orbital description of aromaticity and antiaromaticity.

3.2 Some Selected reactions of aromatic system

Electrophilic aromatic substitution: Gattermann reaction - Gattermann-Koch formylation reaction-Hoeben-Hoesch reaction - Vilsmeir formylation. ***Nucleophilic aromatic substitution:*** Chichibabin amination - Bucherer reaction. ***Transition metal chemistry:*** Pauson-Khand reaction-Heck reaction-Suzuki Coupling - Stille Coupling - Sonogashira Coupling- Negishi cross coupling.

UNIT –IV Organic Stereo Chemistry

4.1 Optical Isomerism

Brief introduction to Chirality: Asymmetry - dissymmetry - chiral axis and chiral plane examples (Biphenyls, Allenes, spiranes and ansa compound, cyclophanes respectively). ***Prochirality:*** Principles of Stereogenecity, stereoselectivity, enantioselectivity, diastereoselectivity. Enantiotopic andDiastereotopic. ***Asymmetric synthesis***: Stereoselective and stereospecific synthesis - stereochemical aspects through various models (Cram / Cram chelation / Felkin-Anh models); Cram's rule. ***Methods of resolution:*** crystal growth - enantiomeric excess.

4.2 Dynamic stereochemistry - Conformational analysis **-** Introduction to terms - conformers, configuration, dihedral angle, torsional strain, conformations.Conformational analysis of cycloalkanes (3,4,5 and 6 membered ring with two substituents). Winstein Eliel equation - Curtin-Hammet principle.

UNIT-V Molecular Rearrangement

5.1 ***Migration of Carbon:*** Wagner-Meerwein rearrangement-Wolf rearrangement-Benzil benzilic acid rearrangement ***Migration to electron deficient nitrogen:*** Hofmann rearrangement - Beckmann rearrangement- Schimdt rearrangement. ***Migration to electron deficient oxygen:*** Bayer villeger oxidation- Dakin reaction.

5.2 ***Migration to electron rich carbon:*** Favorskii rearrangement - Stevens rearrangement - Wittig rearrangement. Neber rearrangement. ***Other rearrangements:*** Dienone-phenol rearrangement - Benzidine rearrangement - Gruvenstein and Zimmermann rearrangements.

Reference Books

1. R. Panico, W.H. Powell, L. Jean,C. Richer, A Guide of IUPAC Nomenclature of Organic compounds, 1993. **(Unit-I)**
2. Jerry March, Advanced Organic Chemistry - Reaction Mechanisms and Structure, John Wiley, New York, 2004. **(Unit-II, III)**
3. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International, New Delhi,2005. **(Unit-IV)**
4. P.S. Kalsi, Stereochemistry, Conformations and Mechanism, New Age International Private Limited, New Delhi, 2004. **(Unit-IV)**
5. Ahluwalia V K, Organic Reaction Mechanism, Narosa Publication, 2010. **(Unit-V)**
6. S.M. Mukherji and S.P. Singh, Reaction Mechanism in Organic Chemistry, Macmillan India Ltd., Patna, 1990. **(Unit-V)**
7. R.S. Cahn and O.C. Dermer, Introduction to Chemical Nomenclature, Butterworths, London, 1979.
8. Peter Sykes, A Guide Gook to Mechanism in Organic Chemistry, Pearson Education, New Delhi, 2004.
9. E.L. Eliel, Stereochemistry of Carbon Compounds, McGraw Hill, New Delhi, 2003.
10. Jonathan Clayden, Nick Greeves, Stuart Warren, Organic Chemistry, Oxford University Press, USA, 2000.

CORE COURSE III : PHYSICAL CHEMISTRY-I

Semester: I **Code : P16CH103**
Credits : 6 **Total Hrs: 90**

General Objectives

1. To know the use of chemical kinetics in understanding the reaction mechanisms and to apply kinetic theories and concepts for homogenous and heterogeneous catalyzed reactions.
2. To understand the behaviour of electrolytes in solution.
3. To know the structure of the electrode surfaces and the application of electrode process.
4. To understand electrode kinetics in comparison with other types of kinetic studies
5. To know the applications of classical thermodynamics in the evaluation of macroscopic properties.

UNIT-I Classical Thermodynamics

Partial molar properties - chemical potential, relationship between partial molar quantities and thermodynamic functions - Gibbs-Duhem equation - calculation of partial molar quantities from experimental data, thermodynamic properties of real gases-activity- fugacity concept - calculation of fugacity of real gas and activity coefficient - definition and experimental determination of activity coefficients of non-electrolytes.

UNIT- II Chemical Kinetics – I

2.1 Theories of reaction rates - simple collision theory - steric factor - ARRT (Eyring's theory) thermodynamic derivation of ARRT-comparison of ARRT with collision theory (A , $\Delta S^{\#}$, E_a and $\Delta H^{\#}$) - kinetic isotope effects.

2.2 Theory of unimolecular reactions-Lindemann's theory - steady state approximation - chain reactions - photochemical reaction between hydrogen and halogens (Cl_2 and Br_2) - gas phase auto-oxidations, explosions-hydrogen-oxygen reaction.

UNIT- III Chemical Kinetics – II

3.1 Application of ARRT to solution kinetics - effects of solvents, double sphere model, effect of ionic strength on ionic reactions - influence of pressure on reaction rates in solution-significance of volume of activation-substituent effects - Hammett and Taft equations.

3.2 Homogeneous catalysis, acid-base catalysis - types and mechanism, derivation of rate law for protolytic acid catalysis and explanation for Arrhenius and van't Hoff intermediates, Bronsted relations - Hammett-Deyrup acidity function - enzyme catalysis - mechanism of single substrate reaction - Michaelis-Menton equation - Influence of pH, concentration and temperature, Line Waver plot and Eddi – Hofstee plot.

3.3 Fast reactions-study of kinetics by stopped flow technique, relaxation methods, T and P jump methods, flash photolysis and magnetic resonance method.

UNIT- IV Electrochemistry-I

4.1 Debye-Huckel-Onsager theory and its derivation -Debye -Falkanhagen and Wein's effects - extension to Debye-Huckel Onsager theory.

4.2 Activity of ions in solutions - mean ionic activity coefficients - experimental determination - Debye-Huckel limiting law - modification for higher concentrations - Bjerrum model.

4.3 Electrochemical cells - Electrode - Electrolyte equilibrium - thermodynamic quantities from emf data - Nernst equation for electrode potential and emf of a cell-classification of electrodes (electrodes of I kind, II kind, redox and membrane) - electrolyte concentration cells (with and without transference) - liquid junction potential - its elimination - applications of concentration cells.

4.4 Electrochemical energy storage systems - primary and secondary cells - fuel cells(efficiency-advantage-types)

UNIT-V Electrochemistry – II

5.1 Electrical double layer - theory of multiple layers at electrode- (Guoy Chapman, Stern and Helmholtz model) - double layer capacity - Electrokinetic phenomena, zeta potential and electro osmotic velocity, zeta potential and streaming potential - determination of zeta potential and interpretation of zeta potential values.

5.2 Process at electrodes-Butler-Volmer equation-high and low field approximation-Tafel equation

5.3 Electrochemical corrosion of metals, constructions and use of Pourbaix and Evans Diagrams and prevention of corrosion.

Reference Books

1. R.P. Rastogi and R.R.Mishra ,An Introduction to Chemical Thermodynamics, Vikas Publishing House, New Delhi, 2000. **(Unit-I)**
2. Philip Mathews, Advanced Physical Chemistry, Foundation books, New Delhi, 2003. **(Unit I-V)**
3. B.R. Puri, L.R.Sharma and M.S. Pathania, Principles of Physical Chemistry, Vishal Publishing Co., Jalandar, 2007. **(Unit-II, III, IV, V)**
4. Peter Atkins and Julio de Paula, Physical Chemistry, Oxford University Press, Oxford, 2002.
5. K.J. Laidler, Chemical Kinetics, Tata McGraw-Hill, New Delhi, 1982.
6. A.A. Frost and R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, New York,1953.
7. I. Amdur and G.G. Hammes, Chemical kinetics - principles and selected topics, McGraw Hill, New York, 1966.
8. G.W. Castellan, Physical Chemistry, Narosa Publishing House, New Delhi, 2002.
9. Robert J. Silbey, Rober A. Alberty, Physical Chemistry, John Wiley & Sons, New York, 2001.
10. Samuel Glasstone, Introduction to Electrochemistry, Prentice Hall, New Delhi, 1975.
11. D.R. Crow, Principles and Applications of Electrochemistry, Chapman and Hall, London, 1988.

CORE PRACTICAL I : INORGANIC CHEMISTRY PRACTICAL – I

Semester: I **Code : P16CH1P1**
Credits : 3 **Total Hrs: 90**

General Objectives

1. To learn to separate and estimate quantitatively metal ions in a binary mixture.
2. To gain skills in synthesizing inorganic complexes.

1. Titrimetry and Gravimetry

Only mixture(s) of solutions should be given for estimation

(i) Cu(V) and Ni (G)
(ii) Cu(V) and Zn (G)
(iii) Fe(V) and Ni (G)
(iv) Zn(V) and Cu (G)
(v) Fe(V) and Zn (G)

2. Preparation of the following complexes:

Tetraamminecopper (II) sulphate
Potassium trioxalatochromate (III)
Potassium trioxalatoaluminate (III)
Tristhioureacopper (I) chloride
Tristhioureacopper (II) sulphate

3. UV – Visible Spectral Studies

Recording UV-visible spectrum of five coordination complexes and interpretation of the spectra (demonstration only).

Reference Book:

1. Jeffery G. Bassett.J, Mendhan, R. C. Vogel's Textbook of Qualitative Chemical Analysis, 5th ed. ELBS, 1989.

CORE PRACTICAL II : ORGANIC CHEMISTRY PRACTICAL – I
(Lab Cum Theory)

Semester: I **Code : P16CH1P2**
Credits : 3 **Total Hrs: 90**

General Objectives

1. To learn the separation techniques of binary organic mixtures and characterize them.
2. To study some single stage preparation of organic compound.
3. To get hands on experience of TLC techniques.

1. Qualitative Analysis of an Organic Mixture Containing two Components

Pilot separation, Semi Micro analysis and derivatization of one of the given components.

Determination of R_f value of both components of the mixture by TLC or PC and identification of the components.

2. Preparation of Organic Compounds (Single Stage)

a) Methyl-m-nitrobenzoate from methylbenzoate
b) Glucose pentaacetate from glucose
c) Resacetophenone from resorcinol
d) Benzophenone oxime from benzophenone
e) p-benzoquinone from hydroquinone

Practical Preparatory Course-1 (Total Hrs30)
Components for evaluation

Test - 1 **Max marks: 30 (Part A 2 X 10, Part B 2x5)**
Test – 2 **Max marks: 30 (Part A 2 X 10, Part B 2x5)**

Course Objective

1. To know the principles behind the Pilot separation of binary mixture and preparation of organic compound.
2. To understand principles behind inorganic volumetric and gravimetric analysis.
3. To learn the principle behind chromatographic techniques.

UNIT 1 Principles behind separation of binary mixture

Solvent polarity - Miscibility of organic compounds in ether / water - principles of solvent extraction - partitioning of solutes - regeneration of organic components and purification and Recrystalisation. Basic steps involved in bulk separation.

UNIT II Principles & Protocols for preparation

Mechanistic details of preparations performed and the conditions to be maintained- green aspects of the preparation - Simple steps for recycling products - Techniques of Recrystalisation.

UNIT III Basic Principles of Inorganic Volumetric and Gravimetric Analysis

Recollection of Concentration terms - Preparation of primary and secondary standards- Types of titrations- Indicators (Redox and internal) - stoichiometry of gravimetric reactions- Common errors in volumetry and gravimetry - methods of reducing errors. Difference between double salts and complexes - protocols and conditions in preparation of complexes- spectral identification of d-d transitions in the complexes prepared (demonstration)

UNIT IV Chromatographic methods

Basic principles of adsorption and partition chromatography - Cautions in preparation and development of chromatograms (both paper and TLC) - Polarity of solvents and elution - Different spotting reagents for identification of organic compounds.

Reference Books

1. Inorganic Semimicro Qualitative Analysis , V.V. Ramanujam, 3rd Edition, The National Publishing Company, Chennai -1, 2004.
2. Organic Chemistry Lab Manual, Gnanaprakasan N.S. & G. Ramamurthy, S. Viswanathan Pvt. Ltd, Chennai -31. 2007.
3. Quantitative Analysis , R.A. Day Jr & A.L. Underwood, sixth edition, PHI Learning Pvt. Ltd., New Delhi, 2009.
4. Systematic Experiments in Chemistry, Arun Sethi, New Age International Pvt. Ltd, New Delhi. 2009
5. N.S.Gnanaprakasam & G. Ramamurthy, Organic Chemistry- Lab Manual , S. Viswanathan Co.Pvt. Ltd.,1998.
6. Vogel's Text book of Practical Organic Chemistry, 4th Edition , ELBS/ Longman, England , 1984.

CORE COURSE IV: INORGANIC CHEMISTRY – II

Semester: II **Code : P16CH204**
Credits : 6 **Total Hrs: 90**

General Objectives

1. To learn CFSE and MO-Theory of co-ordination compounds.
2. To understand kinetic mechanism of reactions which involve co-ordination compounds.
3. To know the photochemical behavior of coordination compounds.
4. To understand the importance of coordination compounds in the emerging field of Photochemistry.
5. To know the applications of coordination compounds in catalysis.

UNIT–I Co-ordination Chemistry

1.1 Nomenclature of mono and polynuclear complexes. Crystal field theory - Splitting of d orbitals in octahedral symmetry - CFSE - strong field and weak field splitting - calculation of CFSE for d^n system. Factors affecting the magnitude of splitting (10Dq). Splitting in tetrahedral symmetry - only weak field splitting - reasons. Tetragonal symmetry - differences between tetrahedral and tetragonal symmetry.

1.2 Jorgensen's relation, Spectrochemical series, Nephelauxetic effect, Jahn-Teller theorem and J-T distortion.

1.3 M.O theory of Octahedral complexes(sigma and pi bonding), M.O theory of tetrahedral and square planar complexes.

UNIT–II

2.1 Kinetics and mechanisms of reactions in solutions

Labile and inert complexes, ligand displacement reactions - Acid hydrolysis, base hydrolysis S_N1CB mechanism and anation reactions in octahedral and square planar complexes-Trans effect- theories and applications. Electron transfer (ET) reactions - electron exchange reactions-complementary and non - complementary types . Types - Inner sphere and Outer sphere processes - Applications of ET reactions in inorganic complexes. Isomerisation and racemisation reactions of complexes - Reactions of the coordinating ligands.

2.2 Stability of Coordination compounds

Stability constants - stepwise and overall formation constants - Factors affecting stability constant- Irving William series- Spectrometric and Jobs methods of determining stability constant.

UNIT–III Inorganic Photochemistry

3.1 Laws of photochemistry- photophysical processes - Jablonski diagram- Fluorosence-phosphoresence- Kasha's rule- Stoke's shift- Types of electronic transitions in metal complexes - Photochemistry of transitions in metal complexes

3.2 Photo-substitution, photo-oxidation, photo- reduction, photo-aquation, photo-isomerization and Unimolecular charge-transfer

3.3 Photochemistry of Cobalt(III) complexes, Ligand field photochemistry of chromium(III) complexes, Adamson's rules, Photochemistry of ruthenium - polypyridine complexes, Photochemistry of organometallic compounds, Reinecke's salt, Chemical actinometer.

UNIT-IV Organometallic Chemistry

4.1. General introduction of organometallic complexes (a) 18-electron compounds (b) 16-electron square planar compounds - Electron count preference- 18 electron rule- (a) neutral-ligand method (b) Donor -pair method. Hapticity - Isolobal Analogy. limitations.

4.2 Structure and bonding of organometallic complexes with various types of ligands such as - carbon monoxide, (Metal Carbonyls) phosphines, Hydrides and d ihydrogen complexes. η^1-alkyl,-alkenyl,-alkynyl,and - aryl ligands. η^2 -alkene (metal olefins Zeise's Salt) - alkyne ligands, non conjugated diene and polyene ligands. Dinitrogen and nitrogen monoxide (metal nitrosyls). The allyl ligand - $\eta^1$and η^3 allyl complexes. Butadiene, cyclobutadiene , cyclooctatetraene, benzene and other arenes Metallocenes-.(a) synthesis and reactivity of cyclopentadienyl compounds (Ferrocene) -(b) bonding in bis (cyclopentadienyl) metal complexes M.O. theory, (c) fluxional behaviour of metallocenes, and (d) bent metallocene complexes

UNIT–V Catalysis in Organometallics

5.1 Catalyst - types of catalyst-catalytic steps - (a)Ligand co-ordination and dissociation-(b) insertion(1,1-migratory insertion reactions) and elimination - (1,2-insertions and β-hydride elimination) (c) nucleophilic attack on co-ordinated ligands (d) oxidation and reduction (e) oxidative addition and reductive elimination.

5.2. Hydrogenation of olefins (Wilkinson's Catalyst) - hydroformylation (Oxo process) - Oxidation of Olefins (Wacker process) - Acetic acid synthesis(Monsanto process) - Polymerisation (Ziegler Natta Catalyst) of alkenes- Oligomerisation - Metathesis - σ bond metathesis, alkene metathesis and Ene-yne metathesis- Fischer -Tropsch Synthesis.

Reference Books

1. James E. Huheey, Ellen A. Keiter and Richard L.Keiter, Inorganic Chemistry, Addison-Wesley, 1993. **(Unit I, II, IV, V)**
2. S. Arunachalam, Photochemistry of inorganic compounds, 2001 **(Unit- III)**
3. D.F. Shriver and P.W.Atkins, Inorganic Chemistry, Oxford, New Delhi, 1999.
4. Keith F. Purcell and John C. Kotz, Inorganic Chemistry, Saundera Goldern Sunburst Series, W.B. Saunders Company, Philadelphia, 1977.
5. J.D. Lee, A New Concise Inorganic Chemistry, ELBS, New Delhi,1995.
6. F. Albert Cotton, Geoffrey Wilkinson and Carlos A. Murillo, Advanced Inorganic Chemistry, John Wiley & Sons, Singapore, 2003.
7. Alan G. Sharp, Inorganic Chemistry, Addison - Weseley, New York, 1999.
8. Gary L. Miessler, Donald A. Tarr, Inorganic Chemistry, Pearson Education, New Delhi, 2004.
9. A. W. Adamson, Inorganic Photochemistry, John Wiley & sons, New York, 2000
10. B.R. Puri, L.R. Sharma and K.C. Kalia, Principles of Inorganic Chemistry - Vishal Publishing Co., Jalandhar, 2007.

CORE COURSE V: REACTIONS AND MECHANISMS IN ORGANIC CHEMISTRY

Semester: II **Code : P16CH205**
Credits : 6 **Total Hrs: 90**

General Objectives

1. To learn reagentless organic reactions.
2. To understand the principle behind thermal and photochemical organic reactions.
3. To know the importance of addition reactions in organic compounds.
4. To learn c-c bond formation reaction in organic synthesis.
5. To study about important oxidizing and reducing reagents in organic synthesis.

Unit I Pericyclic Reactions

1.1 Frontier Orbital Description and correlation approach of Woodward Hofmann rules -Regiochemistry- Stereochemical aspects- Endo/Exo selection - role of secondary orbital interaction in the following: ***The Diels Alder Reactions*** (including 1,3 dipolar additions intramolecular reaction -the retro Diels-Alder reaction- asymmetric Diels-Alder reaction).

1.2 ***Electrocyclic reactions***- Nazarov cyclisation - ***Sigmatropic rearrangements*** (Cope, Claisen, Oxy Cope- aza Cope and Sommelet-Hauser) and Cheleotropic reactions.

Unit II : Organic Photochemistry

2.1 Photo Chemistry- I

Interaction of electromagnetic radiation with matter-Excitation- the excited state- the transfer of excitation energy(sensitization and quenching)- ***photoreduction, photoaddition*** **:** photoaddition of alkene and alkynes to aromatic compounds-photoaddition of alkenene to carbonyl- Norrish type-I&II- photodimerisation, Excimer, Exciplexes, Isomerisation of alkenes- Photostationery state, conjugated dienes and aromatic compounds ***photo oxidation:*** formation of peroxy compounds- oxidative coupling of aromatic compounds.

2.2 Photo Chemistry-II

Intramolecular reactions of carbonyl compound**:** Norrish type I- Norrish type II. - β- unsaturated carbonyl compounds. Intermolecular cyclo addition reactions-[2+2] cycloaddition reactions Paterno - Buchi reaction- cycloaddition reactions of benzene. ***Photo rearrangement:*** cis-trans isomerisation- intramolecular photocyclisation-***sigmatropic rearrangements:*** cyclohexadienone. ***Photo chemical fragmentation*****:** Photolysis of diazoalkanes- alkyl azide.

UNIT III Addition Reactions

3.1 Addition to carbon-carbon multiple bonds-addition mechanisms electrophilic, nucleophilic and free-radical additions-cyclo addition orientation and reactivity. Selected reactions - Birch reduction- catalytic semi reduction of alkynes - Hydroboration-selective hydroborating agents-oxymercuration-demercuration-epoxidation of alkene-Sharpless asymmetric epoxidation- Baeyer Villiger reaction- - Michael reaction.

3.2 ***Addition to carbon-hetero atom multiple bonds-*** addition orientation and reactivity -Selected name reactions - Acyloin ester condensation, Aldol condensation, Benzoin condensation, Cannizaro reaction, Claisen reaction, Darzen's condensation, Knovenegal reaction, Mannich reaction and Stob be condensation.

UNIT-IV Carbon-Carbon Bond Formation Reactions

4.1 Mechanistic details, stereochemical considerations and significance of the following reactions: ***Formation of carbon-carbon single bonds*** - Mitsunobu reaction- Reformatsky reaction - Robinson annulations - Stork enamine alkylation- Gattermann and Gattermann-Kosch formylation reaction. ***Formation of carbon-carbon double bonds***-Bamford-Stevens reaction- Horner-Wadsworth-Emmons reaction- Julia olefination-Perkin reaction. ***Free radical reaction***-Hoffman-Loffler-Freytag reaction- Hundsdiecker reaction

4.2 ***Formation of carbon-carbon single bonds by Organometallic reagents-*** Principles- Organo-lithium compounds -LDA, R-Li- Organomagnesium compounds - Organo copper compounds(Gilman's reagent) - Organo cadmium compounds - Organomercury compounds- Organozinc compounds. ***Reagents containing sulfur, boron, silicon***- sulfur ylide, sulfoxonium ylide, 9-BBN, disiamyl borane, thexyl borane, trimethyl silyl iodide

UNIT-V Reagents for Oxidation and Reduction Reactions

5.1 Preparation, properties and characteristics of the following oxidizing agents and their reaction on alkenes, aromatic rings, ketones, ketals and carboxylic acids - Chromyl chloride, Periodic acid, Pyridinium Chloro Chromate -PCC, Dessmartin, Dichloro Dicyano hydro quinone -DDQ, iodobenzenediacetate, 2- iodoxybenzoic acid - IBX, sodium hypochlorite (bleach), Lead tetra acetate-$Pb(OAc)_4$

5.2 Preparation, properties and characteristics of the following reducing agents and their reactions o n alkenes, alkynes, aromatic rings, carbonyls, Ketals, azo groups, epoxides and carboxylic acids - $LiAlH_4$, Lithium trialkylborohydride, DIBAL, tri-t butyloxyaluminium hydride, $NaBH_4$, sodium cyanoborohydride and hydrazine.

Reference books

1. Ratan Kumar Kar, Frontier Orbital and Symmetry Controlled Pericyclic Reactions, Books and Allied Ltd,2009. **(Unit-I)**
2. Jagadamba Singh, Photochemistry and Pericyclic Reactions, New age, third edition **2012**(UnitI, II)
3. Jerry March, Advanced Organic Chemistry - Reaction Mechanisms and Structure, John Wiley, New York, 2004. **(Unit-III, IV, V)**
4. Richard O.C. Norman, James M. Coxon Principles of Organic Synthesis CRC Press, 1993 **(Unit-III, IV, V)**
5. Jonathan Clayden, Nick Greeves, Stuart Warren, Organic Chemistry, Oxford University Press, USA, 2000
6. James Morris Coxon , Brian Halton, Organic Photochemistry, Cambridge University Press, 2011
7. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press,Cambridge, 1993.

8. Ahluwalia V K, Organic Reaction Mechanism, Narosa Publication, 2010.
9. S.M. Mukherji and S.P.Singh, Reaction Mechanism in Organic Chemistry, Macmillan India Ltd., Patna, 1990

CORE PRACTICAL III : INORGANIC CHEMISTRY PRACTICAL – II (Total Hours: 60)
(Theory and Practicals)

Semester: II **Code : P16CH2P3**
Credits : 3 **Total Hrs: 90**

General Objectives

1. To understand the principles of distribution of common and rare metal ions in different groups.
2. To analyze qualitatively the inorganic mixture containing familiar and less familiar cations.
3. To understand the reactions in the qualitative analysis of rare metal ions in different groups.
4. To imbibe the skill in quantitative estimation of metal ions by colorimetry.

I. Semi micro qualitative Analysis - Analysis of a mixture containing two common and two rare cations.

Common Cations –	I group-Pb, Tl II group - Cu, Cd, Bi ,	III group - Al, Fe,
	IV group - Mn, Zn, Co, Ni,	V group- Ca, Sr, Ba,
	VI group Mg	zero group- NH_4
Rare Cations -	I group - W, Ti , IA group - Se, Te,	II group - Mo,
	III group - Be, Zr, Ce, V, U,	VI group - Li

II. Colourimetric estimation - Estimation of Copper, Ferric, Nickel, Chromium and Manganese using Photoelectric colourimeter.

Practical Preparatory Course -2 (Total Hours: 30)

General Objectives
1. To understand the principles of semi micro qualitative analysis.
2. To learn the principle of error analysis.
3. To know the principle behind colorimetric estimation of metal ions.

Test -1 **Max marks: 30 (Part A 2 X 10, Part B 2 x5)**
Test – 2 **Max marks: 30 (Part A 2 X 10, Part B 2 x5)**

UNIT I Errors in Analysis and Measurements

Chemical analysis- sampling - types of analysis- limitations of analytical methods- accuracy-precision - types of errors- minimization of errors- significant figures- Principles of Organic estimations- Back titrations -Reactions involved in each step of estimation.

UNIT II Good Laboratory Practices

Calibration and use of glass wares- Storing and recycling some reagents in laboratory - Protocols for Handling chemicals and their disposal - Safety measures and first aid in the laboratory- Handling hazards due to strong acids and bases, toxic chemicals, Remedies for Ingestion, Inhalation and direct absorption of chemicals.

UNIT III Principles Of Colorimetric Analysis

A brief recollection of the Laws of Colorimetry - Components and Instruments of a Colorimeter - Mathematical expression and Importance of Absorbance, molar absorptivity - percentage transmittance - Construction of standard graph - extrapolation and interpolation. Preparation of some important organic and inorganic complexing agents.

UNIT - IV Principles of Qualitative Analysis

Rare and common ions - Grouping of ions - principles behind separation of ions into groups - common ion effect - Solubility Product - Group reagents - and reactions involved.

Reference Books

1. V. Ramanujam, Inorganic Semimicro Qualitative analysis, 3rd edition, The National publishing Company, Chennai 1974.
2. Vogel's, Text book of Inorganic Qualitative Analysis, 4th edition. ELBS, 1974.
3. R. Gopalan, P.S. Subramanian, K. Rengarajan, Elements of Analytical Chemistry, Sultan Chand and Sons, New Delhi, 1997

CORE PRACTICAL IV: ORGANIC CHEMISTRY PRACTICALS – II

Semester: II **Code : P16CH2P4**
Credits : 3 **Total Hrs: 90**

General Objectives

1. To learn quantitative analysis in organic chemistry.
2. To get hands on experience on the double stage preparation of organic compounds.
3. To learn the interpretation of UV and IR spectra of organic compounds.

1. Quantitative Analysis of Organic Compounds

Estimation of phenol, aniline, glucose and ethyl methyl ketone

2. Preparation of Organic Compounds: (Double Stage)

a) p-bromo acetanlide from aniline
b) Acetyl salicylic acid from methyl salicylate
c) 1,3,5 - tribromobenzene from aniline
d) p-nitroaniline from acetanilide
e) Benzanilide from benzophenone

3. Interpretation of IR and UV visible spectra of organic compounds (ten in each case).

Reference Books

1. N.S.Gnanaprakasam & G. Ramamurthy, Organic Chemistry- Lab Manual, S. Viswanathan Co. Pvt. Ltd.,1998.
2. Y.R. Sharma & O.P. Vig, Elementary Organic Spectroscopy Principles and Chemical Applications, S.Chand & Co., New Delhi, 2001.
3. Vogel's Text book of Practical Organic Chemistry, 4th edition, ELBS/ Longman, England , 1984.
4. William Kemp, Organic Spectroscopy, Palgrave, New York, 2000.
5. R.M. Silverstein, G.C.Bassier and T.C. Morill, Spectrometric Identification of Organic Compounds, John Wiley Eastern, New Delhi, 1974.
6. J.R. Dye, Application of Spectroscopy of Organic Compounds, Printice Hall, New Delhi, 1965

CORE COURSE VI : ORGANIC SPECTROSCOPY

Semester: III **Code : P16CH306**
Credits : 5 **Total Hrs: 90**

General Objectives

1. To understand the applicability of the spectroscopic techniques
2. To study the structure of the organic compounds from the study of spectra

UNIT–I

1.1 Ultraviolet and spectroscopy

Various electronic transitions (185 - 800 nm), Beer - Lambert Law, effect of solvent on electronic transitions, UV bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Woodward- Fieser rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

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

Definition, deduction of absolute configuration, octant rule for ketones, Cotton effect and ORD curves. Comparison between ORD and CD and their interrelationships.

UNIT– II Infrared Spectroscopy

2.1 Instrumentation and sample handling. Characteristic vibrational frequencies of alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines.

2.2 Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds).

2.3 Effect of hydrogen bonding and solvent effect on vibrational frequencies, over tones, combination bands and Fermi resonance, FTIR.

UNIT–III Nuclear Magnetic Resonance Spectroscopy

3.1 General introduction and definition, chemical shift, spin – spin interaction, shielding mechanism. Chemical shift values and chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four, and five nuclei (first order spectra), virtual coupling, coupling constant.

3.2 Simplification of complex spectra using - nuclear magnetic double resonance, contact shift reagents - solvent effects. Fourier transform technique - Nuclear Overhauser effect (NOE).

UNIT–IV Carbon^{13} NMR Spectroscopy

4.1 General considerations, chemical shift (aliphatic, Olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon)
4.2 Two dimensional NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT, and INADEQUATE techniques.

UNIT–V

5.1 Mass Spectrometry

Introduction, ion production - E1, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

5.2 A review of spectroscopic problems

Calculation of double bond equivalent and its application in structure elucidation. Structure elucidation of organic molecules involving IR, UV, NMR and mass data.

Reference Books

1. P.S. Kalsi, Spectroscopy of Organic Compounds , New Age International , New Delhi, 1998 **(Unit I-V)**
2. Y.R. Sharma and O.P.Vig , Elementary Organic spectroscopy- Principles and chemical Applications, S.Chand & Co., New Delhi,2001. **(Unit I-V)**
3. R.M. Silverstein , G.C. Bassier and T.C. Morrill , Spectrometric identification of Organic Compounds, John Wiley Eastern , New Delhi, 1974
4. J.R. Dyer, Application of Spectroscopy of Organic Compounds, Prentice Hall , New Delhi, 1965
5. W.Kemp , Organic spectroscopy , Palgrave , New York, 2000.

CORE COURSE VII: PHYSICAL CHEMISTRY – II

Semester: III **Code : P16CH307**
Credits : 5 **Total Hrs: 90**

General Objectives

1. To apply the concepts of statistical thermodynamics to study equilibrium reactions and reaction rates.
2. To learn physical and mathematical aspects of quantum mechanics.
3. To solve quantum mechanical problems.
4. To understand and appreciate the quantum mechanical approach to the atomic and molecular electronic structure.
5. To know the limitations of quantum chemistry and classical thermodynamics in the evaluation of macroscopic properties.

UNIT –I Statistical Thermodynamics – I

1.1 Probability - types of events - theories of probability - multiplicative nature of probability - permutations and combinations – Stirling's approximation.

1.2 Statistical mechanics - calculation of thermodynamic probability of system - Assembly ensembles, phase space-definition of micro and macro states - different methods of counting macro and micro states - distinguishable and indistinguishable particles - classical statistics - derivation of Maxwell Boltzmann distribution law- Its application to gaseous system - energy, velocity distribution - concept of negative Kelvin temperature.

1.3 Quantum statistics - Bose Einstein and Fermi Dirac statistics - comparison with Maxwell-Boltzmann statistics - application of BE statistics to photon gas - Application of FD statistics to electron gas and to thermionic emission – derivation of thermionic energy.

UNIT- II Statistical Thermodynamics – II

2.1 Partition function – characteristics - translational, rotational, vibrational, electronic partition function - expression for enthalpy, internal energy, Gibb's energy, entropy (Sackur - Tetrode equation), work function and equilibrium constant in terms of partition functions – partition function of mono atomic and diatomic molecules.

2.2 Heat capacity of solids -Derivation of Einstein equation and its limitations, Debye T - cubed law and its significance.

2.3 Non-equilibrium thermodynamics, steady-state-phenomenological laws and Onsager's reciprocal relations.

UNIT-III Quantum Chemistry-I

3.1 Mathematical concepts for quantum mechanics - differentiation formula for uv, u/v, (u+v), sinx, cosx, and e^x only - partial differentiation - Euler's reciprocal relation, chain rule (statement only) - Integration methods.

3.2 Inadequacy of classical mechanics - wave particle dualism - deBroglie's equation - uncertainty principle - Schrodinger time independent wave quation - significance of ψ and ψ^2-postulates of

quantum mechanics - eigen functions and eigen values - operator algebra - linear and Hermitian, angular momentum operators - commutation relations - orthogonalization and normalization.

3.3 Applications of wave mechanics to simple systems - particle in one and three Dimensional box, Rigid rotator - Harmonic oscillator - rotational and vibrational quantum numbers- zero-point energy.

UNIT- IV Quantum Chemistry – II

4.1 Bohr's correspondence principle - hydrogen atom- shapes and nodal properties of orbitals. Approximation methods - variation method - application to hydrogen and helium atom- perturbation method - application of perturbation theory to helium atom- Hartree Fock Self-consistent field method - many electron atoms- Pauli's principle and Slater determinant.

4.2 LCAO- MO treatment of hydrogen molecular ion and H_2-VB treatment of hydrogen molecule - hybridization of orbitals in BeF_2, BF_3,CH_4. Huckel pi-electron theory and its applications to ethylene butadiene and benzene.

UNIT- V Surface Phenomena

5.1 Adsorption- physisorption and chemisorptions - Langumuir, BET & Gibbs adsorption isotherms- surface area determination - Heat of adsorption, determination. Adsorption from solutions - surface films.

5.2 Surface tension - effect of electrolytes, non electrolytes and surface active agents - micelles and reverse micelles. Solublisation, micro emulsions

5.3 Heterogeneous catalysis - semiconductor catalysis, n-and p-type surfaces - kinetics of surface reactions involving adsorbed species - Langmuir - Hinshelwood mechanism. Langmuir - Rideal mechanism and Rideal - Eley mechanisms.

5.4 Photoelectron Spectroscopy (PES) - principles and techniques of PES, Ultra violet PES, X-ray PES. Application of photoelectron spectroscopy, ESCA and Auger spectroscopy to the study of surfaces.

Reference Books

1. M.C.Gupta, Statistical Thermodynamics, Wiley Eastern Ltd., New Age International, New Delhi, 1998. **(Unit -I, II)**
2. R.P. Rastogi and R.R. Mishra, An introduction to Chemical Thermodynamics, Vikas Publishing House, New Delhi, 2000. **(Unit -I, II)**
3. A.K.Chandra, Introductory Quantum Chemistry, Tata McGraw-Hill, New Delhi, 2003. **(Unit- III,IV)**
4. B.R. Puri, L.R.Sharma and M.S. Pathania, Principles of Physical Chemistry, Vishal Publishing Co., Jalandar, 2007. **(Unit -V)**
5. R. Stephen Berry, Stuart A.Rice and John Ross, Physical Chemistry, Oxford University Press, New York, 2000.
6. D.A. Mcquarrie, J.D. Simon, Molecular Thermodynamics, University Science books, California, 1999.
7. F.W.Sears, Thermodynamics, Kinetic theory of Gases and statistical mechanics, 2nd Edition, Wesley, 1972.

8. Horia Metiu, Physical chemistry- Thermodynamics, Taylor and Francis, 2006.
9. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1998.
10. I.N.Levine, Quantum Chemistry, 5th Edition, Prentice Hall, 2000.
11. R.K. Prasad, Quantum Chemistry, New Age international (P) Ltd., New Delhi, 2002.
12. Peter Atkins and Julio de Paula Atkins, Physical Chemistry, Oxford University Press, Oxford, 2002.
13. G.W.Castellan, Physical Chemistry, Narosa Publishing House, New Delhi, 2002.
14. Robert J. Silbey, Robert A. Alberty, Physical Chemistry, John Wiley and Sons, New York, 2001.
15. P.K. Ghosh, Introduction to Photoelectron spectroscopy, John Wiley and Sons,New York,1989.

ELECTIVE I : ANALYTICAL TECHNIQUES AND 'C' PROGRAMMING

Semester: III **Course Code: P16CH3:1**
Credits : 4 **Total Hours: 75**

General Objectives

1. To learn the principles and operation of various instruments
2. To learn the applications of various electrochemical techniques.
3. To know the fundamentals of C programming language and its application to determine some chemical parameters.

UNIT-I Electroanalytical Techniques

1.1 Cyclic Voltammetry - explanation of the technique, electrodes, a typical cyclic Voltammogram, Eg: electrochemical oxidation of ascorbic acid-reversible and quasi - reversible systems.

1.2 Polarography - Principle and Instrumentation, a typical polarogram, Factors affecting limiting current - residual current, migration current, diffusion current(i_d), Kinetic current, half-wave potential, applications to determine dissolved oxygen, analysis of metal ions in a mixture, estimation of Ni^{2+}.

1.3 Amperometry - Principle, Instrumentation, electrodes, titration curves.

UNIT–II Instrumental Method of Analysis

2.1 Principles and Applications of SEM, TEM and XRD.

2.2 Flow chart diagram of HPLC. Various types - adsorption, partition (reverse phase), partition (normal phase), ion-exchange and size exclusion chromatography - detectors. Interpretation of detector output. Identification of components in a soft drink.

2.3 Gas liquid chromatography - Description of the technique - Schematic diagram of a gas chromatograph, a typical chromatogram, and detectors - flame ionization detector, electron capture detector and applications of GLC.

UNIT-III Fundamentals of 'C' Language

3.1 Structure of a 'C' program - data types, variables, constants, keywords, operators, expression.

3.2 Control structure - if, if-else, nested if-else, while, do-while, for loop, nested for, goto, continue, break, switch case statements (only syntax with simple examples).

3.3 Functions - library function, user defined function. Arrays - definition, initialization, string and character arrays.

UNIT-IV 'C' Programming

4.1 Calculation of reduced mass, molecular weight using sub-routine program,

4.2 Determination of activity coefficient using while loop,

4.3 Calculation of second order rate constant, solving quadratic equation for the calculation of solubility of a sparingly soluble salt,

4.4 Determination of Ea and A using call function.

UNIT -V Data Analysis

Mean, Average, Standard Deviation, Variance and its testing - Correlation and Regression - Least square method for curve fitting.

Reference Books

1. R. Gopalan, P.S. Subramanian, K. Rengarajan, Elements of Analytical Chemistry, Sultan Chand and Sons, New Delhi, 1997.
2 Doughlas A. Skoog, Donald M.West, F. Jeames Holler, Stanley, R. Crouch, Fundamentals of Analytical Chemistry, Thomas Books, Bangalore, 2004.
3 Gary D. Christian, Analytical Chemistry, John Wiley and Sons, Singapore, 2004.
4 B.K. Sharma, Instrumental Methods of Chemical Analysis, Goel Publishing House, Meerut, 1999.
5 H.H. Willard, L.L. Merritt and John A. Dean, Instrumental Methods of Analysis, D. Van Nostrand, New York, 1966.
6. G.L.D. Krupadanam et al., Analytical Chemistry, University Press, Hyderabad,2001.
7. B.R. Puri, L.R.Sharma, Kalia, Advanced Inorganic Chemistry, VishalPublishing Co., Jalandhar, 2007.
8. E. Balagurusamy, Programming in Ansi C, Tata McGraw Hill, New Delhi, 2001.
9. K.V. Raman, Computers in Chemistry, Tata McGraw Hill, New Delhi, 1993.
10. Kishore Arora ,Computer Applications in Chemistry, Anmol Publications, New Delhi, 2004.

ELECTIVE I : GREEN CHEMISTRY

Semester: III **Course Code: P16CH3:2**
Credits : 4 **Total Hours: 75**

General Objectives

1. To learn eco-friendly methods of synthesis.
2. To understand the synthesis of organic compounds with Green Chemistry approach.
3. To know the energy production method from biomass.

Unit - I Principles & Concept of Green Chemistry

1.1 Introduction -Concept and Principles-development of Green Chemistry.

1.2 Atom economy reactions -rearrangement reactions, addition reactions.

1.3 Atom uneconomic-sublimation-elimination-Wittig reactions- Need of Green Chemistry in ourday to day life.

Unit - II Energy Efficient Green Transformations

2.1 Design for Energy efficient transformations - Principles, methodology and examples of the following green reactions: Photochemical reactions- Advantages-Challenge faced by photochemical process.

2.2 Microwave technology on Chemistry- Microwave heating - Microwave assisted reactions-

2.3 Sonochemistry Electrochemical Synthesis-Examples of Electrochemical synthesis. Enzymatic reactions

Unit- III Green Solvents & Catalysts For Synthesis

3.1 Water as the universal Solvent - Aqueous Phase Transformations - Properties, Methods of handling and Applications of the following as solvents for chemical transformations: Ionic Liquids - Super critical Water- Liquid CO_2 - Polyethylene Glycol.

3.2 Green Aspects of Homogeneous and Heterogeneous Catalysis - Use of Phase transfer Catalysts for green synthesis - Solid Phase transformations - Polymer supported reactions - Types of polymer supports - Merrifields Automated synthesis as a typical example of solid supported reactions.

Unit - IV Green Processes in Industries

4.1 Methyl Methacrylate (MMA) - Greening of Acetic acid manufacture-Vitamin C - Leather manufacture -Types of Leather -Difference between Hide and Skin-Tanning -Reverse tanning - Vegetabletanning -Chrome tanning-Fat liquoring.

4.2 Dyeing - Application - Polyethylene - Ziegler Natta Catalysis - Metallocene Catalysis - Eco friendly Pesticides and Insecticides. Some Green

Unit - V Biomass and Measurement of Environmental Performance

5.1 Feed Stocks - Sources - Utilization - Biological Feed Stocks - Fermentation and Plant sources of Chemicals -Glucose and cellulose as feed stock - Conversion of waste to feed stock Biomass -Energy from Biomass.

5. 2 Importance of measurement of environmental performance- lactic acid production-safer Gasoline - introduction to life cycle assessment-four stages of Life Cycle Assessment (LCA) - Carbon foot printing-green process Matrics-eco labels -Integrated Pollution and Prevention and Control(IPPC)- basics of REACH (Registration, Evaluation, Authorization of Chemicals)

Reference Books

1. V.K. Ahluwalia,Methods and Reagents of Green Chemistry: An Introduction by Green Chemistry. www.clri.org **(Unit I-V)**
2. Mike Lancaster , Green Chemistry and Introductory text, II Edition, RSC Publisher,2010
3. P.T.Anastas and J.C Warner, Green Chemistry theory and Practice, Oxford University press, Oxford (1988).
4. P.Tundo et. al., Green Chemistry, Wiley -Blackwell, London (2007).
5. T.E Graedel, Streamlined Life cycle Assessment, Prentice Hall, New Jersey (1998).

CORE PRACTICAL V: PHYSICAL CHEMISTRY PRACTICAL – I

Semester: III **Code : P16CH3P5**
Credits : 3 **Total Hrs: 90**

General Objectives

1. To learn the operations of instruments and data processing.
2. To acquire the skill in evaluation of physical parameters by various methods.

Physical Experiments (Non Electrical)

1. Comparison of strength of acids by the study of kinetics of hydrolysis of an ester.
2. Evaluation of E_a and A by studying the kinetics of acid catalysed hydrolysis of ethyl acetate.
3. Determination of molecular weight by Rast method.
4. Construction of phase diagram of a congruent system.
5. Determination of critical solution temperature of phenol-water system and study of the effect of NaCl on miscibility temperature.
6. Comparison of the strength of acids by the kinetic study of iodination of acetone.
7. Effect of an inert salt on the kinetics of clock reaction between I^- and $S_2O_3^{2-}$.
8. Construction of adsorption isotherm for the adsorption of oxalic acid and charcoal.
9. Polarimetric study of the kinetics of acid catalysed inversion of sucrose.
10. Determination of heat of solution of a substance (benzoic acid or ammonium oxalate) by the measurement of its solubility as a function of temperature.

Reference Books

1. J.N.Gurthu and R.Kapoor, Advanced Experimental Chemistry, S. Chand and Co.,1987.
2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S.Viswanathan and Co.Pvt.,1996.
3. David P.Shoemaker, Carl W.Garland and Joseph W.Nibler, Experiments in Physical Chemistry, 5th Edition, McGraw- Hill Book company , 1989.

CORE PRACTICAL VI : PHYSICAL CHEMISTRY PRACTICAL – II

Semester: III **Code : P16CH3P6**
Credits : 3 **Total Hrs: 90**

General Objectives

1. To analyse and estimate quantitative parameters using some instrumental techniques.
2. To understand the principle and the methodology for qualitative and quantitative estimations

Physical Experiments (Electrical)

1. Conductometric determination of dissociation constant of a weak acid.
2. Potentiometric determination of pK_a of an acid.
3. Measurement of single electrode potentials of Zn^{2+} / Zn and Cu^{2+}/Cu electrodes.
4. Potentiometric estimation of redox titration of $KMnO_4$ with KI or Fe^{2+} or Ce^{4+} and determination of standard redox potential.
5. Potentiometric estimation of mixture of halides.
6. Conductometric estimation of the components of buffer.
7. Conductometric estimation of mixture of weak and strong acids.
8. Conductometric precipitation titration of $BaCl_2$ with $MgSO_4$ and K_2SO_4.
9. Conductometric titration of NH_4Cl and HCl against NaOH.
10. Conductometric titration of mixture of alkali against HCl.
11. Determination of solubility product by
    a) Conductometric method
    b) Potentiometry - Concentration cell method
    c) Potentiometry - Chemical cell method.
12. Potentiometric estimation of mixture of weak and strong acids.
13. Conductometric study of the kinetics of saponification of ester- (Internal/ Demonstration only)

Demonstration experiments using electrochemical analyser.

1. Galvanostatic polariasation measurement of corrosion rate.
2. CV studies of two compounds.
3. Separation of copper and nickel using electrogravimetric method.

Practical Preparatory Course – III (Total Hours: 30)
Components for evaluation

Test -1 **Max marks :30 (Part A 2 X 10, Part B 2 x5)**
Test – 2 **Max marks :30 (Part A 2 X 10, Part B 2 x5)**

Course Objective

1. To learn the principles and methodology of Physical Chemistry Practical

UNIT-I

Preparation of standard solutions- Concentration terms - dilution of solutions- Calculations- Graphs - Regression coefficient-Slope and intercept.

Chemical kinetics- Reaction rates-Reaction molecularities -order of a reaction-Determination of the order of a reaction-Graphical method- Arrhenius equation - The temperature co-efficient-Temperature control using Thermostat.

Principle of Iodination of acetone- Oscillatory reactions - Clock reaction-influence of ionic strength on rate constant.

UNIT-II

Polarimetry - optical rotation -mechanism of inversion of cane sugar.

Thermo chemistry-Heat of formation-Heat of combustion-Heat of solution -integral heat of dilution-heat of hydration. Use of indicators in titrations.

Colligative properties and Phase equilibria - Phase-Component-degree of freedom-Reduced Gibbs phase rule-eutectic temperature-eutectic composition-freezing point diagram of binary mixtures-examples of one, two and three component systems.

Surface phenomenon - differences between adsorption and absorption - adsorbent-adsorbate-Physisorptions-chemisorption-types of adsorption isotherms (Only final equations).

Unit-III

Electrochemistry - Electrical conductance of electrolytes - Specific conductivity - Equivalent conductivity - Molar conductivity- conductance value of ions - Effect of dilution on conductivity.

Ostwald's dilution law-Debye-Huckel Onsager equation- Debye -Huckel limiting law-Kohlrausch law (Only final equation).

Types of conductometric titrations - Standarsiation of conductometer - Wheatstone's meter bridge-Conductivity cell - Advantages of conductometric titrations.

Concept of solubility- Solubility Product - Common ion effect - pH scale - Buffer.

Potetiometric titrations- Galvanic cell- Nernst Equation - Electrode potential- Electrochemical series-Types of electrodes- salt bridge- liquid junction potential- standardization of potentiometer- Standard cell and Western cell. Measurement of EMF of cell-overall cell reactions - writing cell diagram - Applications of potentiometric titrations.

Reference Books

1. Jagadamba singh, R.K.P. Singh, Jaya Singh, L.D.S Yadav, I.R. Siddiqui and Jaya Shrivastava, Advanced Practical Chemistry, Pragati Prakasham Publishers, 5th Edition, **2014**.
2. B.Viswanathan and P.S. Raghavan, Practical Physical Chemistry, Viva Books Pvt.Ltd, **2006**. **(Unit I-III)**
3. B. Yadav, Advanced Practial Physical Chemistry, Satyendra Rastogi Mitra, 34th edition, 2014.
4. David P. Shoemaker, Carl-W.Garland and Joseph W. Nibler, Experiments in Physical Chemistry, Mc Graw-Hill-International, 5th Edition, 2004.

Project Preparatory Course
Components for evaluation

Test -1 **Max marks :30 (Part A 2 X 10, Part B 2 x5)**
Test – 2 **Max marks :30 (Part A 2 X 10, Part B 2 x5)**

General Objectives

1. To know the importance of review of literature.
2. To understand the basic requirements of a project work and plan ahead of the project work.
3. To learn the methodology of thesis writing.

UNIT I Research Methodology

The Know how's of Research - General Objectives - Types of research - Steps involved in research - Identifying a problem for project- Evolving strategies for solving - Designing feasible experiments - planning and scheduling a Project

UNIT II Review of Literature

Sources of literature- primary - secondary - tertiary - importance and characters of Monographs, Journals, Notes and Communications. Methods of literature survey - Chemical Abstracts and Indexing – Computer aided searches - Use of Search engines and advanced searches using Google Scholar - PubMed, RSC, PDB. Ordering and scheming the literature review - Identification of gaps in literature

UNIT III Preparation of a Project Report and Presentation

Planning a project report - criteria for selection of the titles and subtitles - Scientific language for writing – Tenses and voices for the Introduction - Review and Report. Language editors and raters and their usage- Bibliography preparation - styles and types - Methods of including references in MsWord - Mendeleev and Microsoft End note for reference. Simple tips for usage of MS word, Excel, power point, Origin and OneNote for project report preparation

References

1. P Ramadass and A. Wilson Aruni, Research and Writing across the disciplines , MJP Publishers, Chennai, 2009.
2. https://www.mendeley.com/download-mendeley-desktop/
3. http://cassi.cas.org/
4. https://www.cas.org/
5. J.N.Gurthu and R.Kapoor, Advanced Experimental Chemistry, S. Chand and Co.,1987.
6. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II),S.Viswanathan and Co.Pvt.,1996
7. David P.Shoemaker, Carl W.Garland and Joseph W.Nibler, Experiments in Physical Chemistry, 5th Edition, McGraw- Hill Book company, 1989.

CORE COURSE VIII : INORGANIC CHEMISTRY – III

Semester: IV **Code : P16CH408**
Credits : 5 **Total Hrs: 90**

General Objectives

1. To know the applications of electronic spectroscopy to study the structure of molecules.
2. To gain knowledge about the principles of NMR, EPR, Mossbauer spectroscopy.
3. To analyze qualitatively the spectrum of certain chemical compounds.
4. To interpret the given spectra to elucidate the structures of the molecules.

Unit- I Electronic Spectroscopy

1.1 Electronic Spectroscopy of complexes- characteristics of d-d transitions, selection rules for d-transitions - Term symbols for d - ions, Use of Orgel diagrams for d^{1-10} octahedral and tetrahedral complexes.

1.2 Tanabe-Sugano diagrams for $d^1$and d^6 octahedral complexes only. Effect of Jahn-Teller distortion and spin - orbit coupling on spectra. Charge transfer spectra (LMCT and MLCT).

1.3 Intensity of Charge transfer transitions in inorganic and coordination compounds, Electronic absorption spectra of low spin and strong field complexes.

Unit- II IR and Raman Spectroscopy

2.1 Combined uses of IR and Raman Spectroscopy in the structural elucidation of simple moleculesn like H_2O, ClF_3, NO_3^-, and ClO_3^-.

2.2 Effect of Co-ordination on ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulphoxide.

2.3 Effect of isotopic substitution on the vibrational spectra of molecules. Differentiation of coordinated water and lattice water. Applications of IR to identify terminal and bridging carbonyl group.

UNIT- III NMR SPECTROSCOPY

3.1 Applications of NMR to inorganic compounds - (spin-spin coupling involving different nuclei ^1H,^{31}P,^{13}C) NMR of metal hydrides(H^1NMR) - Metal carbonyls (C^{13} NMR) - F^{19}, P^{31}NMR.

3.2 Effect of quadrupolar nuclei (^2H,^{10}B,^{11}B) on the ^1H NMR spectrum.

3.3 NMR of paramagnetic molecules -isotopic shifts, contact and Pseudo-contact interactions-lanthanide shift reagents.

UNIT- IV EPR SPECTROSCOPY

4.1 Basic principle - characteristics of 'g' - Hyperfine splitting - selection rules - factors affecting the magnitude of the 'g' values. 'g' value of transition metal ions - dependence on spin - orbit coupling and crystal field effects.

4.2 EPR of d^1 to d^9 systems of first transition series. Tetragonally distorted copper complexes - Zero-field splitting and Kramer's degeneracy.

4.3 Solid state EPR - spin-lattice relaxation - spin-spin relaxation - exchange processes.

UNIT-V

5.1 Magneto-chemistry

Determination of magnetic susceptibility by Guoy and Faraday methods. Magnetic properties of low spin and high spin octahedral complexes of first row transition metals - Curies law, Curies-Weiss law, Curie temperature and Neel temperature, Types of Magnetism - Paramagnetism, Diamagnetism, Ferro and anti-ferromagnetism.

5.2 Mossbauer Spectroscopy

Principle - Doppler effect - Recoil energy - isomer shift - quadrupole effect - magnetic interactions - magnetic field on spectra -simple applications to iron and tin compounds.

Reference Books

1. B.K. Sharma, Spectroscopy, Krishna Prakashan, New Delhi, 1993. **(Unit I-V)**
2. P.S. Sindhu, Molecular Spectroscopy, Tata McGraw Hill, 2000.
3. H. Kaur, Spectroscopy, Pragati Publications, Meerut,2001.
4. V.B.Pathania, Spectroscopy, Campus Books, New Delhi,2002.
5. R.S. Drago, Physical Methods in Inorganic Chemistry, East West Publishers, New Delhi, 1965.
6. EAV Ebsworth, Structural Methods in Inorganic Chemistry, ELBS, Oxford,1988.
7. A. Abdul Jameel, Application of Physical Methods to Inorganic compounds, JAN publication, Trichy, 2003.
8. James E. Huheey, Ellen A. Keiter and Richard L Keiter, Inorganic Chemistry, Addison Wesely,1993.

CORE COURSE IX : PHYSICAL CHEMISTRY- III

Semester: IV **Code : P16CH409**
Credits : 5 **Total Hrs: 90**

General Objectives

1. To learn the symmetry operations, point groups of molecules and to apply the fundamentals of group theory for spectroscopic selection rules.
2. To know quantization of energy and the interaction of electromagnetic radiation with matter.
3. To study the fundamentals of molecular spectroscopy.
4. To understand the mathematical foundations of different branches of spectroscopy.
5. To know the application of spectroscopy to study the structure of molecules.

Unit-I Group Theory

1.1 Group theory - theory of group - symmetry of elements and symmetry of operations, point groups of molecules, properties of a group and sub-group, isomorphism, cyclic, abelian, class - similarity transformation and conjugate, matrix representation - product of symmetry operations, group multiplication tables(C_n, C_{nv} and D_{nh} only) - great orthogonality theorem and its consequences, construction of character tables(C_{2V} and C_{3V}). Direct products – reducible and irreducible representation - Wave function as bases for irreducible representation.

1.2 Crystal point group, crystal symmetry - screw axis and glide plane, space groups, translational elements of symmetry differences between molecular symmetry and crystal symmetry.

Unit – II Applications of Group Theory

2.1 Group theory and molecular electronic states - Transition moment integral - spectroscopic selection rules to IR, Raman (H_2O, NH_3, trans-N_2F_2) and electronic spectroscopy (HCHO) .

2.2 Projection operators and their use to construct SALC - evaluation of energies and MO's for systems - ethylene, butadiene and benzene, hybridization schemes of orbitals - (sp, sp^2 and sp^3)

Unit-III Molecular Spectroscopy-I

3.1 Introductory aspects: electromagnetic radiation - representation of spectra, the line width and intensity of spectral transitions - factors influencing them- Einstein's transition probability and oscillator strength.

3.2 Infrared spectroscopy: Selection rules -harmonic and anharmonic oscillations - rotation and vibrational spectra of polyatomic molecules - CO_2,H_2O - fermi resonance - influence of rotation on the spectra of diatomic molecules - parallel and perpendicular bands.

3.3 Raman spectroscopy: Raman effect - elastic and inelastic scattering - quantum theory - origin of Stokes, antiStokes and Rayleigh lines - selection rules - rotational and vibrational Raman spectra - simple molecules (CO_2, H_2O), mutual exclusion principle - Basics of Laser Raman spectroscopy.

Unit-IV Molecular Spectroscopy-II

4.1 Electronic spectra: electronic spectra of molecules, Born Oppenheimer approximation, vibrational coarse structure - Frank-Condon principle, dissociation energy, predissociation rotational fine structure of electronic vibrational transitions - Fortrat diagram- various types of transitions - auxochromes , chromophores - bathochromic and hypsochromic shift.

4.2 Emission spectroscopy: fate of electronically excited molecules- fluorescence, phosphorescence, emission spectra of molecules.

4.3 Photochemistry: Differences between photochemical and thermal reactions - Quantum yield- Photophysical processes in electronically excited molecules - Jablonski diagram-energy transfer processes - Radiative and Non-Radiative transitions - Fluorescence-relation to structure- Phosphorescence- conditions for Phosphorescence emission (spin-orbit coupling)- Photosensitization - Stern - Volmer equation and its applications- Chemiluminescence.

Unit-V Molecular Spectroscopy-III

5.1 NMR spectroscopy : Energy of interaction and its derivation, Zeeman effect, nuclear spin and applied magnetic field, Effect of 'B' on splitting - Larmor precession and its expression - relaxation processes - PMR - chemical shift - factors affecting chemical shift and coupling constant (J) - spin-spin interaction - FT-NMR - C^{13} NMR spectroscopy - chemical exchange - Problems.

5.2 NQR spectroscopy: characteristics of quadrupolar nucleus - effect of field gradient and magnetic field upon quadrupolar energy levels - NQR transitions - applications of NQR spectroscopy.

5.3 Lasers: Nature of stimulated emission- coherence, monochromaticity, population inversio - cavity and mode characteristics - types of lasers- solid state, gas, chemical and dye lasers.

Reference Books

1. K.V. Raman, Group Theory and its Application to Chemistry, Tata McGraw-Hill, New Delhi, 2000. **(Unit I, II)**
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall, New Delhi, 2002. **(Unit III, IV, V)**
3. P.K. Ghosh, Introduction to Photoelectron spectroscopy, John Wiley and Sons, New York, 1989. **(Unit IV)**
4. F.A. Cotton, Chemical Applications to Group Theory, John Wiley and Sons, New York, 2003.
5. Robert. L. Carter, Molecular symmetry and Group Theory, John Wiley and Sons, New York, 1998.
6. B.E. Douglas and C.A. Hollingsworth, Symmetry in bonding and spectra- an introduction, Academic Press, 1985.
7. Robert J. Silbey, Robert A. Alberty, Physical Chemistry, John Wiley and Sons, New York, 2001.
8. W.Kemp, Organic Spectroscopy, 3rd Edition. McMillon, 1994.
9. W.Kemp, NMR Spectroscopy, 3rd Edition. Mc Millon, 1994.
10. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw-Hill, New York, 1964
11. D.L. Andrews, Lasers in Chemistry, 3rd edition, Springer-Verlag, London, 1997.

12. C.N. Banwell and E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th edition, Tata McGraw-Hill, New Delhi, 2000.
13. K.V. Raman, R. Gopalan and P.S. Raghavan, Molecular Spectroscopy, Thomson and Vijay Nicol, Singapore, 2004.
14. I.N.Levine, Molecular Spectroscopy, John Wiley and Sons, New York, 1974.
15. A.Rahman, Nuclear Magnetic resonance- Basic Principles, Springer-verlag, New York, 1986.
16. R.S. Drago, Physical methods in chemistry, Saunders, Philedephia, 1977.
17. B.R. Puri, L.R.Sharma, M.S. Pathania, Principles of Physical Chemistry, Vishal Publishing Co., Jalandhar, 2007.
18. Walter J. Moore, Basic Physical Chemistry, Prentice-Hall, New Delhi, 1986.
19. G.W. Castellan, Physical Chemistry, Narosa Publishing House, New Delhi, 1986.
20. I. N. Levine, Physical Chemistry, Tata McGraw-Hill, New Delhi, 2002.
21. K.K. Rohatki-Mukherjee, Fundamentals of Photochemistry, New Age International, New Delhi, 1997.
22. A. Singh and R. Singh, Photochemistry, Campus Books, New Delhi, 2005.

ELECTIVE II: PRINCIPLES AND APPLICATIONS OF DRUG DESIGN AND DISCOVERY

Semester: IV **Code : P16CH4:2**
Credits : 4 **Total Hrs: 60**

General Objectives

1. To understand drug design and discovery.
2. To learn the different types of active sites of enzyme and their interaction with drug molecule.
3. To understand basic principles of retro-synthesis.
4. To know fundamentals of computer aided drug designing.

Unit I Drug Design and Discovery

Historical background - drug targets: lipids, carbohydrates, proteins, enzymes, and nucleic acids as drug targets and receptors. Receptor Pharmocology -Agonists and Antagonists(partial and full) - Allosteric Modullators - Pharmacokinetics and pharmacodynamics: administration, absorption, distribution, metabolism, elimination of drugs - bioavailability of drugs - side effects - Case study : serotonin and dopamine receptors and transferring drugs.

Unit II Drug Identification and Validation

Steps in drug discovery - Leads identification - Hits - Drug validation - Natural products as drugs - molecular recognition in drug design - thermodynamic considerations - physical basis and inter molecular interactions between drugs and targets like electrostatic interactions - ionic bonds - hydrogen bonds - Inductive interactions - dispersive forces. Stereochemistry in drug designing - stereospecificity of drug targets - Eudesmic eudismic ratio - Examples of Eutomers and Distomers

Unit III Retrosynthetic Strategies for Drug Synthesis

Introduction to retrosynthetic analysis and disconnection approach - synthons acceptor and donor - synthetic equivalents - umpolungs - planning a synthesis - relay and convergent routes- Guidelines for disconnection - one group C-X and C-C disconnections - Chemoselectivity. Two group C-C disconnections in dicarbonyls - Case Study : Synthesis of Amelfolide.

UNIT IV Computer Aided Drug Design

Molecular modeling in drug design - Energy Minimization methods - both Molecular Mechanics and Quantum mechanical Methods - Energy minimization - Conformational analysis - Structure based and Ligand based Drug design - QSAR - parameters - Quantitative models of QSAR - Hansch methods - free Wilson model -3D pharmacophore modeling - Docking - rigid and flexible methods of docking - Prediction of Binding modes - Protein Ligand binding free energies - Docking Score - validation.

Unit V Quantum Mechanical Methods

Electronic structure calculations - Geometry Optimization - Potential Energy Surface - Global and Local Minima - Identification of Transition states - Semiemperical and Density Functional Methods - Calculation of atomic Charges, Electrostatic Potential Maps.

Reference Books

1. Andrew R. Leach, Valerie J Gillet, An Introduction to Cheminformatics, Revised Edition, Springer, Netherland, 2007. **(Unit I, II, IV, V)**
2. Stuart Warren **,** Organic Synthesis The Disconnection Approach, Wiley; 2nd edition (December 31, 2008) **(Unit III)**
3. Larsen et al, Text book of Drug design and Discovery, 4th Edition, London and Newyork , Taylor and Francis, 2004.
4. Graham L. Patrick, An Introduction to Medicinal Chemistry, 4th Edition, Oxford University Press,2009.
5. Johann Gasteiger, Thomas Engel, Chem-informatics : A Textbook, Wiley VCH, Weinheim, 2003.

ELECTIVE III : BIO-INORGANIC CHEMISTRY

Semester: IV **Code : P16CH4:3**
Credits : 4 **Total Hrs: 75**

General Objectives

1. To know the role of coordination compounds in living systems.
2. To understand the chemistry of bio-molecules.

Unit-I

1.1 An overview of metals in Biology - Essential metals - their fate and conversion in Biological systems. Bio- organo metallic chemistry - Metal ion Complexation - Thermodynamics and Kinetics - Electron transfer reactions.

1.2 Biological role of alkali metals - Alkali and alkaline earth metals complexes: Complexes of β-diketone, crown ethers, cryptands and spiranes; Template Effect, macro-cyclic effect , macro-cyclic effect.

Unit-II Transport of Metals

Structure, characteristics and composition of cell membrane - The fluid model - Membrane Transport: Active and passive transport, Ping-Pong model of facilitated diffusion- Iono-phores, Transporter proteins- Ion pumps - Mechanism of Na^+ and K^+ pumps - Gated transport -voltage gated transport. Types of ports in ion transport - uniport- symport - Antiport. Gap Junctions

Unit III Redox Systems in Biology

3.1 Bio-Redox agents:Fe-S proteins - Ferredoxin and Rubredoxin, HIPIPs - Functions and Structure , Non-heme iron proteins (Ferritin, Hemosiderin)

3.2 Metals as Carriers - Iron Containig Oxygen Carriers - Myoglobin - Hemoglobin - Structure and Prosthetic group - Mechanism of reversible binding of dioxygen and Cooperativity -CO binding to Fe and model Complexes containing Cobalt.

3.3 Oxygen uptake proteins: Cytochrome P-450 enzyme.

3.4 Photosynthesis - Light phase and dark phase reactions, Photosystem I and II. Nitrogen Fixation - Invivo Copper proteins: Blue copper proteins(Cupredoxins) -Type I-Plastocyanin - Type III-Hemocyanin. Non blue copper proteins - TypeII-Galactoseoxidase and Superoxidase dimutase .Some other copper protein -Ceruloplasmin.

Unit IV Metal Dietary Requirement And Toxicity

4.1 Minerals in Diet - Requirement of various minerals in Physiological and biochemical functions- Classification of minerals according to their functions in the body - Digestion and Absorption of minerals - Mechanism of Iron Absorption - Ferroprotein secretion.
4.2 Toxicity Due to Metals - Bio-chemistry of toxic metals Pb, Cd, Hg, Al, Fe, Cu, Pu - Detoxification by metal chelates.

Unit–V Metals in Medicine

Structure, Mode of action, Bio – availability and solubility and advantages and side effects of the following drugs and therapies:

5.1. Cancer therapy: Cis-platin and its mode of action

5.2. Radiotherapy: Radio-pharmaceuticals- Technetium. Chemotherapy - basics and applications

5.3. Anti rheumatic agents: Gold containing drugs and their action.

5.4. Psychopharmacological drugs: Lithium drugs and their mode of action.

5.5. Contrast enhancing agents for MRI: MRI imaging, Synthesis of Gadolinium based contrast agents.

Reference Books

1. Asim. K. Das. Bio-Inorganic chemistry, Books and Allied Publishers, 2007. **(Unit I-IV)**
2. Subbiah Balaji, Nanobiotechnology, MJP Publishers, Triplicane, Chennai, 2010. **(Unit -V)**
3. Puri, Sharma, Kalia, Advanced Inorganic chemistry, Vishal publishing Co., Jalandhar, 2007.
4. Stephen J. Lippard, Jeremy Mark Berg, Principles of Bioinorganic Chemistry, University Science Books, 1994

ELECTIVE IV: COMPUTATIONAL CHEMISTRY AND DRUG DESIGNING PRACTICAL

Semester: IV **Code : P16CH4:P**
Credits : 2 **Total Hrs: 45**

General Objectives

1. To develop programming skill in C
2. To learn the basic skills in drug designing using QSAR technique
3. To understand the applications of software packages for computations in chemistry

Theory for Internal evaluation

Components for evaluation

Test -1 **Max. marks : 30 (Part A 2 X 10, Part B 2 x5)**
Test – 2 **Max. marks : 30 (Part A 2 X 10, Part B 2 x5)**

Fundamentals of 'C' Language

Structure of a 'C' program - data types, variables, constants, keywords, operators, expression. Control structure - if, if-else, nested if-else, while, do-while, for loop, nested for, go to, continue, break, switch case statements (only syntax with simple examples). Functions - library function, user defined function. Arrays - definition, initialization, string and character arrays.

No Viva-voce for External Examination

List of Experiments

1. Using the pre-processor and macro concepts, write a program to calculate the energy of a non-rigid rotator using the formula Energy = hc $[BJ(J+1)-DJ^2(J+1)^2]$
2. Using the while loop write a program to calculate the mean activity ($f\pm$) coefficient of 3 uni-univalent electrolytes using the formula $\ln f \pm = -2.303 |Z^+Z^-|C$
3. The solubility of a salt S in the presence of a common ion of concentration Y is related to solubility product by $S(S+Y) = Ksp$. Write a program to solve the quadratic equation

   $S^2 + SY - Ksp = 0$ to obtain solubility S.

4. The dissociation constant of acetic acid is related to the degree of dissociation α by the

   Formula $$K = \frac{\alpha^2 C}{(1-\alpha)}$$

   Write a program to calculate the value of K for 10 values of concentration using do While loop and also calculate the average value for the dissociation constant.

5. The Arrhenius equations at two different temperature (T_1 and T_2) with rate constants k_1 and k_2 are given.

   $$\ln K_1 = \ln A - \frac{Ea}{RT_1} \qquad \ln K_2 = \ln A - \frac{Ea}{RT_2}$$

   Solve these two simultaneous equations and find the unknown energy of activation (E_a) and frequency factor (A).

6. Using the switch control statement, calculate the rate constant for zero order, first order and second order reaction.

7. Building small molecules using Argus Lab and Spartan Calculation of Electronic structure Properties

8. Docking: Small molecule docking using Argus Lab.

9. QSAR a) Calculation of Clog P values
   b) Effect of functional group on activity
   c) Drawing QSAR plot based on the QSAR results.

Reference Books

1. E. Balagurusamy, Programming in Ansi C, Tata McGraw Hill, New Delhi, 2001.
2. K.V. Raman, Computers in Chemistry, Tata McGraw Hill, New Delhi, 1993.
3. Kishore Arora , Computer Applications in Chemistry, Anmol Publications, New Delhi, 2004.
4. Andrew R. Leach, Molecular modeling Principles & Applications, Prentice Hall, 2nd edition, 2008.

Project
Project: 15 Hrs.(Sem.III) + 75 Hrs (Sem IV)

Semester: IV **Code : P16CH4PJ**
Credits : 4 **Total Hrs: 90**

INTERNAL: EXTERNAL – 60:40

General Objective

To get trained in applying the knowledge and skills to solve a problem, give inferences and record the findings as a scientific report.

Components for internal evaluation

- Preparation of report(20 marks)
- Innovation in choice of problem (20 marks)
- Skills in systematic analysis and recording.(20 marks)
- Regularity and involvement(20 marks)
- Viva - voce (20 marks)

**** Internship:**

2 Extra credits can be earned by attending Summer/ Winter internships on submission of attendance certificate and project report.

ELECTIVE : ANALYTICAL TECHNIQUES IN CHEMISTRY

Credits : 4 **Total Hrs: 75**

General Objectives

1. To learn the importance of pesticides and fertilizers
2. To understand the chemistry of soil and coal analytical techniques
3. To know the concepts of clinical analysis
4. To analyze soil and coal samples

Unit-I Analysis o Pesticides and Fertilizers

***1.1 Pesticides*:** General introduction, analysis of pesticides in general with reference to DDT, Dieldrin,Malathion, Parathion, BHC by different analytical methods such as titrimetric, colorimetric, chromatography and electroanalytical methods.

***1.2 Fertilizers*:** Sampling and sample preparation, determination of water, total nitrogen, urea, total phosphates, potassium, acid or base forming quality.

Unit-II Soil Analysis and Coal Analysis

***2.1 Soil analysis*-** Classification and composition, pH and conductivity, analysis of constitutents such as nitrogen, phosphorous, potassium and microconstitutents (Zn and Cu).

***2.2 Coal analysis*-** Proximate analysis (moisture content, ash content, volatile matter, fixed carbon).Ultimate analysis (carbon, hydrogen, sulphur, nitrogen, oxygen content). Combustion of carbonaceous fuel- Flue gas. Calorific value and its units, Bomb calorimeter.

Unit-III Corrosion and Corrosion Analysis

3.1 Definition, draw backs and theories of corrosion-dry and wet corrosion, Different types of corrosion-Pit, Soil, chemical and electrochemical, intergranular, waterline, microbial corrosion.

3.2 Measurement of corrosion by different methods, factors affecting corrosion, passivity, galvanic series, protection against corrosion

Unit-IV Radioanalytical Techniques

4.1 Neutron sources, Neutron activation analysis, principle, methodology and application for trace analysis.

4.2 Isotope dilution analysis-principle and application, radioactive dating based on carbon-14 and lead isotopes.

Unit-V Clinical Analysis

5.1 General composition of blood, Collection and storage of blood samples

5.2 Qualitative tests for reducing sugar. Estimation of blood glucose, urea, uric acid, blood urea-nitrogen, total serum protein, serum albumin, serum creatinine, serum phosphate, serum bilirubin, serum cholesterol.

Reference books

1. Gunter Sweig. Analytical Methods for pesticides and plant growth regulators and food additives, Vol.II , Academic Press, London.2002.
2. B. K. Sharma ,Industrial chemistry, Krishna Educational Publishers, 16th edition, 2014
3. Alka L. Gupta, Analytical chemistry, Pragati Prakashan, 2014.,
4. O.P. Vermani and A. K. Narula, Applied Chemistry-Theory and Practice, New Age International Ltd, 2012.
5. V. M. Balsaraf, Applied Chemistry I and II, I K International Publishers, 2010.

ELECTIVE: RADIATION CHEMISTRY

Credits : 4 **Total Hrs: 75**

General Objectives

1. To learn the basics of radiation chemistry.
2. To understand the principles and working of radio analytical techniques
3. To comprehend the applications of radiations in pharmaceuticals.

Unit-I Radiation Chemistry

1.1 Measurement of dose. Dosimetric terms and units (Roentgen, REM, Rad, Gray, Sievert), inter conversions.

1.2 Calculation of absorbed dose-various types of dosimeters, chemical dosimeters (Fricke, Ceric sulphate and FBX), experimental methods, TLD badges, Radiolysis-definition, process,

Unit II Radiolysis

2.1 Radiolysis of water and aqueous solutions, hydrated electron.

2.2 Effect of radiation on biological substances, genetic effects, radiation effects on organic compounds (Halides-carboxylic acids), polymers, nitrates and solid thermoluminescence.

Unit-III Radioanalytical Techniques

3.1 Neutron sources, Neutron activation analysis, principle, methodology and application for trace analysis.

3.2 Isotope dilution analysis-principle and application, Isotopic exchange reaction, mechanism and application in use of radioisotopes and tracers, radioactive dating based on carbon-14 and lead isotopes.

Unit – IV Radioimmunoassay

4.1 Radioimmunoassay (RIA), discovery, principle, set up of RIA

4.2 Principle of Immunoradiometric assay (IRMA), principle and set up

UNIT – V Radiopharmaceuticals

5.1 Radioimmunoassay (RIA), discovery, principle, set up of RIA, Principle of Immunoradiometric assay (IRMA), principle and set up.

5.2 Radiopharmaceuticlas, classification of products, preparations, qualitycontrol aspects, 99Mo-99mTc generator, Cylotron based products, PRT studies.

Reference books

1. Robert J. Woods, Alexei K. Pikaev, Applied Radiation Chemistry: Radiation Processing, Publisher, Wiley inter-science , 1993.
2. B.K. Sharma, Nuclear and Radiation Chemistry, Krishna Prakashan Media(P) Ltd, 2000.
3. Mazumder, Fundamentals of Radiation Chemistry, Academic Press, 1999.

ELECTIVE : NATURAL PRODUCTS CHEMISTRY

Credits : 4 **Total Hrs: 75**

General Objectives

1. To understand the classification of natural products
2. To learn the structural morphology of biomolecules

UNIT –I Classification of Natural Products:

1.1 Chemical structure, classification, structure elucidation based on degradative reactions.

1.2 Isolation and structural elucidation of selected alkaloids and terpenes - quinine, morphine, and reserpine.

UNIT – II Amino Acids

2.1 Synthesis of amino acids - reactions - properties - amino acids in nature - amino acids and their metabolites in nature .

2.2 Structure of proteins - peptides, insect pheromones.

UNIT-III Steroids

3.1 Classification - synthesis and structural elucidation of cholesterol.

3.2 Conversion of cholesterol to progesteron -anderosterone and testosterone -cortisone - vitaminD .

UNIT –IV Nucleic Acids

4.1 Structure of nucleosides and nucleotides - RNA and DNA, complimentary base pairing.

4.2 Watson and Crick model. DNA-drug interaction.

UNIT- V Carbohydrates

5.1 Determination of configuration - Hudsons rules - structure of sugars - transformation of sugars, 5.2 Preparation of alditols, glycosides, deoxysugars. Synthesis of vitamin C from glucose.

Reference books

1. I. L. Finar, Organic Chemistry Vol. I & Vol. II- Pearson Education, 6th edn.
2. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Part A & B, 3rd Edition, Part B. Plenum/Rosetta, 1990.
3. I. Fleming, Selected Organic Synthesis, John Wiley and sons, 1982.
4. Atta-ur-Rahman, Studies in Natural Products Chemistry, Vol.1 and 2, Elsevier, 1988.

ELECTIVE : CHEMISTRY OF POLYMERS

Credits : 4 **Total Hrs: 75**

General Objectives

1. To know the chemistry of polymerization
2. To understand the concept of molecular designing

Unit – I Concept of Macromolecules

1.1 Principle of duality and molecular design - tetrahedral model of product development. Nomenclature and classification.

1.2 Raw material for the synthesis of polymers. Synthetic schemes. Petroleum and petrochemicals - Naphtha as a source of petrochemicals.

Unit – II Polymerization Processes

2.1 Free radical addition polymerization - kinetics and mechanism. Chain transfer. Molecular weight distribution and molecular weight control.

2.2 Cationic and anionic polymerization: Kinetics and mechanism. Living polymers. Step growth polymerization.

2.3 Linear Vs cyclic polymerization. Other methods of polymerization - bulk, solution, melt, suspension, emulsion and dispersion techniques.

Unit - III Polymer Stereochemistry

3.1 Configuration and conformation. Tacticity. Chiral polymers. Polymer characterization. Molecular weights - Methods for determining molecular weights - static, dynamic, viscometry, light scattering and GPC.

3.2 Crystalline and amorphous states. glassy and rubbery States. Glass transition temperature and crystalline melting of polymers.Degree of crystallinity - X-ray diffraction. Thermal stability of polymers.

Unit - IV Polymer Solutions

4.1 Flory-Huggins theory. Chain dimension - chain stiffness. End-to-end chain distance of polymers. Conformation - random coil, solvation and swelling.

4.2 Determination of degree of cross linking and molecular weight between cross links. Industrial polymers - synthesis, structure and applications of industrially important polymers.

Unit-V Specialty Polymers

5.1 Polymers as aids in organic synthesis. Polymeric reagents, catalysts , substrates. Liquid crystalline polymers - Main chain and side chain liquid crystalline polymers.

5.2 Phase morphology. Conducting polymers - Polymers in optical lithography - Drug delivery - Drug carriers .

Reference books

1. F.W. Billmayer, Textbook of Polymer Science. 3rd Edn, Wiley. N.Y. 1991.
2. J.M.G Cowie, Polymers: Physics and Chemistry of Modern Materials. Blackie. London, 1992.
3. R.J.Young, Principles of Polymer Science, 3rd Edn. , Chapman and Hall. N.Y. 1991.
4. P.J. Flory, A Text Book of Polymer Science. Cornell University Press. Ithacka, 1953.
5. F. Ullrich, Industrial Polymers, Kluwer, N.Y. 1993.
6. H.G.Elias, Macromolecules, Vol. I & II, Academic, N.Y. 1991.

PG - Non Major Elective Courses (NMEC)
(Offered to Students of other Disciplines)

Semester	Course	Code	Title	Hrs./ Week	Credits	Marks		
						CIA	ESA	TOTAL
II	NMEC-I	P16CH2E1	Chemistry for Healthy living	4	2	25	75	100

NMEC COURSE I : CHEMISTRY FOR HEALTHY LIVING

Semester: II **Code : P16CH2E1**
Credits : 2 **Total Hrs: 60**

General Objectives

1. To know the role of chemistry in diet.
2. To learn to identify harmful components in personal care products.

UNIT-I

1.1 Food

Source of energy - Calorie -Requirements - Constituents of food Balanced diet - Mal-nourishment, Obese.

1.2 Diseases due to food stuffs - Food Poisoning and First aid to food poisoning.

UNIT-II

2.1 Proteins

Types of proteins - Classification based on structure, composition - Amino acids as building blocks - protein energy inter relationship - function of protein in the body - denaturation and renaturation. Milk proteins - plant proteins and egg proteins - recommended allowances in food.

2.2 Carbohydrates

Classification of Carbohydrates - Basic Structure of a few sugars and their Importance -Change of Carbohydrates on Cooking - Caramelization- recommended allowances in food.

UNIT-III

3.1 Fats: Types of fats in food, lipids body constituents - food stuffs with fat - Iodine value, Saponification value and R.M. value of oils- Lipids and relation with atherosclerosis. Importance of fat, dietary fat, Lipid profile – HDL, LDL, Cholesterol.

3.2 Vitamins

Sources, requirement - deficiency diseases - decomposition and losses during cooking- recommended allowances in food.

UNIT-IV

4.1 Minerals

Mineral in Food - Principal minerals elements functions - (Deficiency and daily requirements) - Na, Cl, Mg, Fe, Cu, Mo, Zn, Cr, V, Co, Mn, I,S,K, and P.

UNIT-V

5.1 Cosmetics and Personal Care

Basic ingredients, additives and flavoring used in agents soaps, tooth pastes, lipsticks, perfumes, colognes, deodorants and antiperspirants.

5.2 Harmful beautifying practices and their chemistry -(Keratin depletion in hair-coloring - cleaning and curling of hair).

5.3 Basic tests for identifying good and bad cosmetics - pH Test.

Reference Books

1. Seema Yadav, Food Chemistry, Anmol Publishing (P) Ltd., New Delhi, 2000. (**Unit I-IV)**
2. Alex V. Ramani, Food Chemistry, MJP publishers, Chennai, 2009.**(Unit I-IV)**
3. Carl H. Snyder, The Extraordinary Chemistry of Ordinary things, John Wiley and Sons Inc., New York, 1992. **(Unit - V)**
4. N. Krishnamoorthy, K. Jeyasubramanian and P. Valli Nayagam, Applied Chemistry, Tata Mc Graw Hill, New Delhi, 1999.