

PG & RESEARCH DEPARTMENT OF CHEMISTRY

JAMAL MOHAMED COLLEGE (AUTONOMOUS), TIRUCHIRAPPALLI – 20

PG COURSE STRUCTURE FROM 2011-12

SEM	SUBJECT CODE	COURSE	SUBJECT TITLE	HRS / WEEK	CREDIT	INT. MARK	EXT. MARK	MARK
I	11PCH 1401	CORE-I	Inorganic Chemistry-I	6	4	25	75	100
	11PCH 1402	CORE-II	Organic Chemistry-I	6	4	25	75	100
	11PCH 1403	CORE-III	Physical Chemistry-I	6	4	25	75	100
	11PCH 1404:P	CORE-IV	Inorganic Chemistry Practical-I	6	4	40	60	100
	11PCH 1405:P	CORE-V	Organic Chemistry Practical-I	6	4	40	60	100
TOTAL				30	20	155	345	500
II	11PCH 2406	CORE-VI	Inorganic Chemistry-II	6	5	25	75	100
	11PCH 2407	CORE-VII	Organic Chemistry-II	6	5	25	75	100
	11PCH 2408	CORE-VIII	Physical Chemistry-II	6	5	25	75	100
	11PCH 2409:P	CORE-IX	Inorganic Chemistry Practical-II	6	5	40	60	100
	11PCH 2410:P	CORE-X	Organic Chemistry Practical-II	6	4	40	60	100
TOTAL				30	24	155	345	500
III	11PCH 3411	CORE-XI	Inorganic Chemistry-III	6	5	25	75	100
	11PCH 3412	CORE-XII	Organic Chemistry-III	6	5	25	75	100
	11PCH 3413:P	CORE-XIII	Physical Chemistry Practical-I	6	5	40	60	100
	11PCH 3501	CORE BASED ELECTIVE-I	Pharmaceutical Chemistry	6	4	25	75	100
	11PCH 3502	CORE BASED ELECTIVE-II	Analytical methods in Chemistry	6	4	25	75	100
TOTAL				30	23	140	360	500
IV	11PCH 4414	CORE- XIV	Physical Chemistry-III	6	5	25	75	100
	11PCH 4415:P	CORE-XV	Physical Chemistry Practical-II	6	5	40	60	100
	11PCH 48	PROJECT WORK	Project	6	5	25	75	100
	11PCH 4503	CORE BASED ELECTIVE-III	Special Topics in Chemistry	6	4	25	75	100
	11PCH 4504	CORE BASED ELECTIVE-IV	Instrumentation Techniques	6	4	25	75	100
TOTAL				30	23	140	360	500
GRAND TOTAL				120	90	590	1410	2000

UNIT – I

(18)

- 1.1 **Ionic Bond and Crystal Structure:** Radius ratio rules – Calculation of limiting ratios for Coordination Number 3 to 6. Classification of ionic structures - AX type (ZnS, NaCl, NiAs, CsCl) and AX₂ type (CaF₂, TiO₂, CdI₂), (structures only).
- 1.2 Defects in crystals : Schottky and Frankel defects - Metal excess defects. F - Centre. Metal deficiency defects – Positive ion deficiency – extra interstitial negative ions. Semiconductors, transistors and rectifiers, photovoltaic cells, superconductors.
- 1.3 Lattice energy – Born - Lande equation derivation - significance

UNIT – II

(18)

- 2.1 **Covalent and Coordinate Bonds:** M.O. theory – Symmetry and overlap – construction of molecular orbitals in homo and hetero nuclear diatomic molecules. Electron density contour diagrams in H₂ and F₂. Comparison of V.B and M.O theories. Linnet's double quartet theory.
- 2.2 Crystal field theory – Splitting of d-orbitals in O_h summary – Strong and weak fields – CFSE – Calculation. Splitting in T_d symmetry and tetragonal symmetry. Differences between symmetries - Jahn Teller distortion - splitting pattern in square planar. Factors affecting the magnitude of 10 Dq. Nature of the ligands – Spectrochemical series, Jorgensen's relation. Pi bonding and M.O. theory – Ligands with filled and empty pi orbitals – effects on 10 Dq. Nephelauxetic effect – Magnetic Properties.

UNIT – III

(18)

- 3.1 **Complexes of π - acceptor ligands:** Carbonyls – 18 e⁻ rule – preparation, properties and structures of simple and poly nuclear carbonyls. Carbonylate anions, carbonyl anions, carbonyl hydrides, isolobal fragments – Nitrosyl Complexes – Preparation. Bridging and terminal nitrosyls, bent and linear nitrosyls. Dinitrogen and dioxygen complexes.
- 3.2 **Carbon π - donor Complexes:** Synthesis, Structure and bonding of alkene, alkyne and allyl complexes. Metallocenes – Stability and Reactivity. Molecular orbital concept of metallocenes – derivatives.

UNIT– IV

(18)

- 4.1 **Nuclear Chemistry:** Radioactivity - Modes of radioactive decay - α , β and γ decay, orbital electron capture, nuclear isomerism, internal conversion.
- 4.2 **Detection and determination of radioactivity:** Cloud chamber, Nuclear emulsion, Proportional Counter, Geiger - Muller Counter – Scintillation and Cherenkov Counter. Particle accelerators: Linear, Cyclotron, Synchrotron, Betatron and Bevatron - Nuclear reactors.
- 4.3 **Nuclear Reactions:** Transmutation, Stripping and pick - up, Fission, Fusion, Spallation and fragmentation reactions. Scattering reactions – Sources of neutrons – Neutron activation and isotopic dilution analysis – applications of radioactive isotopes.

UNIT –V

(18)

Acids and bases:

- 5.1 Protonic acids - Proton affinities - Differentiating and leveling solvents – Hammett H_0 scale - Acidic behavior of the binary hydrides – co-solvating agents – Oxyacids - Organic acids - acetic acid and the inductive effect, aromatic acids and resonance effects - hydrolysis and aquoacids - amphoteric oxides - non-protonic concepts of acid base reactions – Lux-Flood concept - Usanowich concept. Hard and soft acids and bases - Classification of acids and bases as hard or soft - acid and base strength of hardness and softness – Symbiosis - theoretical basis of hardness and softness - electro negativity of hardness and softness.
- 5.2 **Non-aqueous solvents:** liq. NH_3 , CH_3COOH , BF_3 , N_2O_4 , HF and SO_2 .

REFERENCES:

1. J.D. Lee – “A new concise Inorganic Chemistry”, 5th Ed., ELBS, 2005.
2. G. Friedlander, J.W. Kennedy and J.M. Miller – “Nuclear and Radiochemistry”(2000).
3. Cotton and Wilkinson – “Advanced Inorganic Chemistry”, 6th Ed., John Wiley & Sons, New York- 2004.
4. James E. Huheey, Ellen A. Keiter and Richard L. Keiter – “Inorganic Chemistry Principles of Structure and Reactivity”, 4th Ed., Pearson Education –sixth impression - 2009.
5. H.J. Arnikaar – “Essential of Nuclear Chemistry”, 4th Ed., Wiley Eastern Limited, 2001.
6. E.A.V. Ebsworth, W.H. Rankin, Cradock – “Structural Methods in Inorganic Chemistry”, ELBS, 1987.
7. Bodie E. Douglas and Darl H. McDaniel, Concepts and models of Inorganic Chemistry, 3rd Wiley India Pvt. Ltd. New Delhi, 2002.
8. Maheswar Sharon & Madhuri Sharon – “Nuclear Chemistry” Ane books Pvt.Ltd, New Delhi -2009.

UNIT – I

(18)

Nomenclature and reaction intermediates

- 1.1 Nomenclature of organic compounds – IUPAC nomenclature of linear and branched alkanes, alkenes, polyenes and alkynes with and without functional groups - Naming of heterocyclic compounds having not more than two hetero atoms such as oxygen, nitrogen and sulphur – Nomenclature of alicyclic, bicyclic and tricyclic compounds with and without single functional group.
- 1.2 Reaction intermediates: Free radicals, carbenes, nitrenes, carbanions and carbocations – generation, stability, structure and reactivity – non-classical carbocations.
- 1.3 **Heterocyclic Compounds:**
Synthesis and reactions of azoles – Imidazole, Oxazole and Thiazole.
Synthesis and reactions of Azepine, Oxazine, Thiazine and Pyrazine.

UNIT – II

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Organic Stereochemistry – I

- 2.1 Optical Isomerism – Principle elements of symmetry – concept of chirality – Newmann, Sawhorse and Fisher Projection formulae – representation and interconversions. Optical isomerism of lactic and Tartaric acids – Configurational nomenclature – D and L,R and S notations of acyclic and cyclic chiral compounds – Stereochemistry of allenes, spiranes, and biphenyls. stereogenic centre. Definition of Prochirality – Asymmetric synthesis – Cram's Rule – Prelog's Rule.
- 2.2 **Dynamic stereochemistry:-**
Quantitative correlations between conformation and reactivity. Weinstein-Eliel equation – Curtin-Hammett principle – Conformation and reactivity of mono and di substituted cyclic systems – Saponification of ester – Esterification of an alcohol – Chromic acid oxidation of cyclohexanols – Neighbouring group participation – Deamination of 2-amino cyclohexanol – Sharpless asymmetric epoxidation – stereospecific and stereoselective reactions.

UNIT – III

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3.1 Aromaticity of compounds:

Definition of aromaticity – Huckel's and Craig's Rules – ring currents – Non-benzenoid aromatic compounds – Aromatic character in 3,5 and 7 membered ring compound – Anti-aromaticity – systems with 2,4,6,8,10,14 and 18 electrons - Azulene - Annulenes – Sydnones – Alternant and non alternant hydrocarbons. Homoaromaticity.

3.2 Elimination Reaction :

E1, E2, E1CB and Ei mechanisms – Stereochemical aspects of elimination reactions – Elimination Vs substitution reactions – Bredit's rule - Chugaev reaction – dehydration of alcohols – dehydrohalogenation – Hoffmann degradation – Cope elimination.

UNIT – IV

(18)

4.1 **Methods of determining reaction mechanism:**

Energy profile diagrams - Thermodynamic and kinetic control of organic reactions – intermediate versus transition state - isotope effects – kinetic and non – kinetic methods of determination of reaction mechanisms – product analysis and its importance – cross over experiment – isotopic labelling studies – stereo chemical studies.

4.2 **Correlation analysis:** Linear free energy relations – Hammett equation – significance of sigma and rho – applications, deviations and limitations – Taft equation and applications.

UNIT – V

(18)

Natural Products:

5.1 **Carbohydrate:** Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, sugar methyl ethers and acid derivatives of sugars, polysaccharides of industrial and biological importance, dextrin, chemistry of sialic acids, cell-cell recognition and blood group substances. Configuration and conformation of glucose, fructose and maltose – photosynthesis of carbohydrates.

5.2 **Nucleic acids:** Chemistry of nucleic acids – structure and properties - biological implication and replication of DNA and RNA – types of RNA and their functions.

5.3 **Terpenoids:** Structural elucidation and synthesis of α -Pinene, Camphor, Zingiberene, Farnesol and Squalene.

REFERENCES:

1. R. Panico, W.H. Powell, L. Jean, C. Richer, “A guide of IUPAC nomenclature of organic compounds”, (1993).
2. Jerry March – “Advanced organic chemistry reactions mechanism and structure”, 4th Ed., (2006), Wiley India Pvt. Ltd.
3. F.A. Carey and R.J. Sundberg – “Advanced organic chemistry” Vol. I and II– 3rd Ed., (1984), Plenum Publications.
4. Raj. K. Bansal – “A Text Book of Organic Chemistry” Revised 4th Ed., (2005), New Age International Publishers Ltd., New Delhi.
5. Raj. K. Bansal – “Heterocyclic Chemistry”, 4th Ed., (2005), New Age International Publishers Ltd., New Delhi.
6. P.S. Kalsi – “Stereochemistry conformation and Mechanism”, 6th Ed., (2005), New Age International Publishers Ltd., New Delhi.
7. Ernest. Eliel and Samuel H. Wilen – “Stereochemistry of Organic Compounds” – Wiley Student Ed., (2006). John Wiley and Sons Pvt. Ltd., Singapore.
8. T. Nasir Puri – “Stereochemistry of Organic Compounds”, Revised Ed., (2005), Wiley Eastern Ltd.
9. I.L. Finar – “Stereochemistry and the Chemistry of Natural Products”, Vol-2, 5th Ed., (2006). Dorling Kindersley (India) Pvt. Ltd.
10. Peter Sykes – “A Guide Book of Reaction Mechanism”, 5th Ed., (2005).
11. Gurdeep Chatwal – “Organic Chemistry of Natural Products”, Vol. I & II, Revised 5th Ed., (2005), Himalaya Publishing House.
12. P.N. Mukerjee – “ a text book of organic reaction, mechanism ” Dominant Publishers and Distribution Pvt. Ltd, New Delhi, 2011.

UNIT - I (18)**Introduction to Classical Mechanics and Exact Quantum Mechanical Result**

- 1.1. Classical mechanics – General principles, basic assumptions, postulates of classical mechanics, conservation laws, D'Alembert's principle, Lagrange's and Hamilton's equations of motion (no derivation).
- 1.2. Operators- algebra of operators, commutation relations, commutators, linear, angular momentum, Laplacian, Hermitian, Hamiltonian and Ladder operators, eigen values and eigen functions, Hermitian property of operators, orthogonality and normalization.
- 1.3. Postulates of quantum mechanics – discussion of the Schrödinger wave equation to simple systems viz., particle in a box – one and three dimensional, quantum numbers, harmonic oscillator – zero-point energy, Bohr's Correspondence principle, rigid-rotator, Hydrogen and hydrogen like atoms (He^+ and Li^{2+}), significance of n , l and m , shapes of atomic orbitals – radial and angular probability distribution functions.

UNIT - II (18)**Application of Quantum Mechanics to Multielectronic Systems**

- 2.1. Approximation methods - linear variation principle, application to hydrogen and helium atoms, perturbation method for non degenerate systems, application of perturbation theory to helium atom,
- 2.2. Two electron systems – symmetric and antisymmetric wave functions, spin of electrons and Pauli's principles and Slater determinant, self consistent field theory - Hartree-Fock Self Consistent field theory, Slater type orbitals – slater rules, orbital energies.
- 2.3. Theory of chemical bonding (diatomic molecules) – Born-Oppenheimer approximation, LCAO – MO and VB treatments of the hydrogen molecule, Huckel molecular orbital (HMO) theory and its applications to conjugated systems – ethylene, allyl radical and butadiene(linear) principle of hybridization – sp , sp^2 and sp^3

UNIT-III (18)**Theory of spectroscopy:****IR spectra:**

- 3.1. Einstein coefficient of absorption and transition probabilities – basis of selection rules – representation of spectra – the width and intensity of spectral lines – oscillator strength.
- 3.2. Vibration spectra – selection rules – harmonic and anharmonic oscillators – hot band, overtones – Fermi resonance, combination bands, rotation – vibration spectra of diatomic molecules – transition for the rigid rotor – coupling of rotation and vibration – linear and perpendicular bands – PQR branches – FT-IR spectroscopy.

3.3 Raman Spectra:

Raman Effect – elastic and inelastic scattering – selection rules – pure rotational and rotational-vibrational Raman spectra – polarization of light and Raman Effect – mutual exclusion principle – Fermi resonance – laser Raman spectroscopy.

UNIT – IV

(18)

THEORY OF NMR-I

- 4.1 Behavior of a bar magnet in a magnetic field – Magnetization vectors – resonance condition – relaxation process – Bloch equation – chemical shift and its measurement.
- 4.2 Scalar Spin - Spin Coupling Mechanism – Nature of the Coupling, Direct Dipolar Coupling – NMR in Solids – magic angle spinning – nuclear magnetic resonance imaging (NMRI) – principles and applications
- 4.3 FT-NMR – Principle, Measurements of T_1 by FTS, Use of T_1 for peak assignment.

UNIT – V

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THEORY OF NMR-II

- 5.1 Second Order Spectra – Introduction, More Complicated Second Order System, Double Resonance and Spin Tickling Experiments - Introduction, Spectral Simplification,
- 5.2 Evaluation of thermodynamic data with NMR – Rate constants and activation enthalpies from NMR – Determination of reaction orders by NMR – some application of NMR kinetic studies.
- 5.3 Two dimensional NMR –Theory of 2D NMR(preliminary)

REFERENCES

- 1. F.L.Pillar, Elementary Quantum Chemistry, McGraw Hill, 1970
- 2. A.K.Chandra, "Introductory Quantum Chemistry" 4th edition; Tata – McGraw Hill, 2010.
- 3. R.K.Prasad, Quantum Chemistry, New Delhi, Wiley-Eastern Ltd, 1992.
- 4. Rusell S.Drago, Physical Methods in Chemistry, W.B.Saunders Company.
- 5. C.N.Banwell and E.M.Mccash , Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill Publishing Company Limited, New Delhi, 2009.
- 6. Manas Chanda, Structure and Chemical bonding including molecular spectra, Tata McGraw-Hill Publishing company Ltd., New Delhi-2.
- 7. S.C.Rakshit,Physical chemistry, seventh edition – Sarat book distributors, Kolkata, 2004.
- 8. G.Aruldhass, Molecular structure and spectroscopy, second edition, PHI learning Pvt. Ltd., New Delhi, 2008.
- 9. David.W.Ball, Physical Chemistry, Cengage Learning India Pvt. Ltd., New Delhi, 2009.

UNIT – I

(18)

- 1.1. **Reactivity of Complexes** – Kinetics and Mechanism of reactions in solutions- Labile and inert complexes – Ligand displacement Reactions – hydrolysis – acid & base, aquation in O_h complexes. Electron Transfer Reactions, complementary and non-complementary types – inner and outer sphere processes – Isomerism in square planar complexes – Trans effect – Theories and Applications. Template effect and synthesis of macrocyclic ligands.
- 1.2. **Stability of coordination compounds:** Detection of complex formation in solution, stability constants, stepwise and overall formation constants pH metric, polarographic and photometric methods of determining formation constants- factors affecting stability – statistical and chelate effects.

UNIT – II

(18)

- 2.1. **Organometallic Chemistry:** 16 and 18 electron rules - Catalysis by Organometallics- Ligand association and dissociation – oxidative addition and reductive elimination – insertion reactions – reactions of coordinated ligands in organometallics – Hydrogenation, hydroformylation, polymerisation of alkenes, olefin oxidation (Wacker Process), Fischer – Tropsch synthesis, epoxidation, metathesis.
- 2.2. **Oxygen Transport and energy transfer of metals proteins:** Hemoglobin and myoglobin – Oxygen transport and storage. Electron transfer and Oxygen activation. Ferredoxins and rubredoxines – Copper proteins – classification – Electron transfer, oxygen transport. Oxidases and reductases – cytochrome oxidase – superoxide dismutase. (Cu, Zn), Urease and hydrogenases.

UNIT-III

(18)

- 3.1. **Electronic spectroscopy:** Electronic configuration - Terms, states and microstates of atoms and ions – Derivation of term symbols (p^2 and d^2) and arranging the various term according to their energies - spectroscopic terms – L-S coupling and jj coupling – effect of interelectronic repulsion and spin-orbit coupling – Racah parameters B and C – selection rules and the breakdown of selection rules – mixing of orbitals.
- 3.2. Orgel diagram – characteristics – prediction and assignment of transitions for d^n weak field systems. Tanabe – Sugano diagrams – prediction and assignment of transitions for weak field and strong field – d^n systems - band intensity, band width - band shape-calculation of β and $10 Dq$ for simple octahedral complexes of Co and Ni- charge transfer spectra.

UNIT-IV

(18)

- 4.1. **IR and Raman spectroscopy:** Combined use of IR and Raman spectroscopy in the structural elucidation of N_2O , H_2O , ClF_3 , NO_3^- , ClO_3^- - Effect of coordination on ligand vibrations – use of group vibrations in the structural elucidation of metal complexes of urea, cyanide, nitrate and sulphate – Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal complexes.
- 4.2. **Mossbauer Spectroscopy:** Mossbauer transition and Doppler Effect – isomer Shift quadrupole effect – magnetic effect on spectra – simple application to iron and tin compounds.
- 4.3. **Lanthanides:** co-ordination compounds of lanthanides - spectral and magnetic properties.
- 4.4. **Actinides:** synthesis of elements –magnetic and spectral characteristics of actinides.

UNIT – V

(18)

- 5.1. **Extraction and Uses of Metals:** Metallurgy of Zr, Ge, Be, Th, U –Preparation and uses of their important compound.
- 5.2. **Inorganic chains:** Catenation, heterocatenation – silicate minerals (names and structure only) Intercalation chemistry – talc, muscovite (structure only)
- 5.3. **Rings:** Preparation and Structure of Borazines & Phosphazenes – Craigg and Paddock model - Dewar model – Preparation and Structure of sulphur-nitrogen ring system (S_4N_4 , $\text{N}_4\text{S}_4\text{F}_4$)

REFERENCES:

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter – “Inorganic Chemistry Principles of Structure and Reactivity”, 4th Ed., pearson Education –sixth impression -2009.
2. A. Abdul Jameel – “Application of Physical Methods to Inorganic Compounds”, Jan Publications, (2007).
3. A.D.P. Lever, Inorganic Electronic Spectroscopy, 2nd Edition, Elsevier, London, 1984.
4. Nakamoto, Infrared spectra of coordination compounds.
5. S.J. Lippard and J.M. Berg – Principles of Bioinorganic Chemistry: Panima Publishing Company, New Delhi, 1997.
6. W. Kaim and B. Schwederski – Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life: John Wiley & Sons, New York, USA, 2001.
7. Cotton and Wilkinson – Advanced Inorganic Chemistry, 5th Edn.: Wiley Interscience Publication, John Wiley & Sons, New York, USA,2000.
8. Cotton and Wilkinson – “Advanced Inorganic Chemistry”, 6th Ed., John Wiley & Sons, New York- 2004.
9. R.H. Crabtree – The Organometallic Chemistry of the Transition Metals: John Wiley & Sons, New York (2000).
10. S.E. Kegley and A.R. Pinhas – Problems and Solutions in Organometallic Chemistry: University Science Books, Oxford University Press,2002.
11. P. Powell – Principles of Organometallic Chemistry, 2nd Edn.: Chapman and Hall, London,2003.
12. B. Douglas, D.H. McDaniel and J.J. Alexander – Concepts and Models of Inorganic Chemistry, 2nd Edn.: John Wiley & Sons, New York,2005.
13. E.A.V. Ebsworth, W.H. Rankin, Cradock – “Structural Methods in Inorganic Chemistry”, ELBS, 1987.

UNIT – I

(18)

- 1.1 **Aliphatic nucleophilic substitution:**
SN₁, SN₂ and SN_i mechanisms – effect of substrate structure, leaving group, attacking nucleophiles and solvent – neighbouring group participation – substitution at allylic carbons and vinylic carbons - Ambident nucleophiles.
- 1.2 **Aliphatic Electrophilic substitution :**
SE₁, SE₂ and SE_i mechanisms – effect of substrate structure, leaving group, attacking electrophiles and solvent –Stork - Enamine reaction, Halogenation of aldehydes and ketones.
- 1.3 **Aromatic nucleophilic substitution:**
Unimolecular, bimolecular and benzyne mechanisms, Zeigler alkylation, Sandmayer and Chichibabin reactions.

UNIT – II

(18)

- 2.1 **Reduction reactions:**
Reduction reactions with LiAlH₄, NaBH₄, tritertiary butyloxy aluminium hydride, sodium cyano borohydride, trialkyl tin hydride, lithium di isopropyl amide, DIBAL, 9-BBN and diisopinocampheyl borane. Gilman's reagent, Hydrazines, MPV reduction, Clemmensen reduction and Wolff-Kishner reduction, Birch reduction.
- 2.2 **Oxidation reactions:** Oxidation with chromyl chloride, periodic acid, selenium dioxide, lead tetraacetate, Osmium tetroxide and H₂O₂ - Oppanauer oxidation.

UNIT- III

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- 3.1 **Addition reactions:**
Addition to carbon – carbon multiple bonds – Electrophilic addition, nucleophilic and free radical additions, orientation and reactivity, Hydroxylation, Hydroboration, Expoxidation, Diel's – Alder reaction. Michael addition, Ozonolysis, 1,3 – dipolar addition reaction- Stereo chemical studies in addition reactions, wherever applicable.
- 3.2 **Name reactions:**
Mannich, Cannizaro, Crossed Cannizaro, Dieckmann, Stobbe, Benzoin, Grignard reactions - Darzen's Glycidic ester condensation and Wittig reaction.

UNIT – IV

(18)

- 4.1 **Molecular rearrangements:**
Wagner – Meerwin, Dienone – Phenol, Wolff, Lossen, Schmidt, Benzidine - Bayer–Villiger, Stevens, Claisen, Fries, Cope, Wittig and Favorski.
- 4.2 **Carotenoids:** Introduction – Classification, structural elucidation of β- carotene, α- carotene, lycopene and xanthophylls.
- 4.3 **Peptides:** Modern methods of peptide synthesis with protection and deprotection, Merrifield resin, Solid phase synthesis, combinatorial synthesis of peptides, Chemistry of oxytocin, valinomycin, enkephalins, self assembly and Aggregation of peptides.

5.1 **Steroids:**

Classification – Structural elucidation of cholesterol (synthesis not required) – Structural elucidation and synthesis of vitamin D, Oestrone, progesterone, ergosterol, stigmasterol and equilenin. Conformation of steroids – Biosynthesis of cholesterol

5.2 **Vitamins:**

Physiological importance – Classification, occurrence, chemistry of Vitamins A, C and E, structure elucidation and synthesis, deficiency syndromes.

5.3 **Lipids:** Classification and biological importance of fatty acids and lipids.**REFERENCES:**

1. Jerry March – “Advanced organic chemistry reactions mechanism and structure”, 4th Ed., (2006), Wiley India Pvt. Ltd.
2. F.A. Carey and R.J. Sundberg – “Advanced organic chemistry” Vol. I and II– 3rd Ed., (1984), Plenum Publications.
3. S.P. Shukla and G.L.Trivedi – “Modern Organic Chemistry”, Millinium Ed., (2000) Rajendra Ravidra Printers Pvt. Ltd., New Delhi.
4. Raj. K. Bansal – “A Text Book of Organic Chemistry”, Revised 4th Ed.,(2005), New Age International Publishers Ltd., New Delhi.
5. Jagadamba Singh and Jaya Singh – “Photochemistry and Pericyclic Reactions” Revised 2nd Ed., New Age International Publishers Ltd., New Delhi,2000.
6. I.L. Finar – “Stereochemistry and the Chemistry of Natural Products”, Vol-2, 5th Ed., (2006). Dorling Kindersley (India) Pvt. Ltd.
7. R.O.C. Norman – “Principles of Organic Synthesis” – 2nd Ed., (1986), Chapman and Hall Publications, New York.
8. O.P. Agarwal – “Reactions and Reagents in Organic Chemistry”, 5th Ed., (2005), Goel Publishing House, Meerut.
9. J.N. Gurtu and R.Kapoor – “Organic Reactions and Reagents”, 1st Ed., (1988), Sultan Chand Company Pvt. Ltd.
10. Gurdeep Chatwal – “Organic Chemistry of Natural Products”, Vol. I & II, Revised 5th Ed., (2005), Himalaya Publishing House.
11. Dr.Ratan kumar kar, “Redox reagents in organic synthesis”, Vol.I,2009, New central book agency (p) Ltd, Kolkata.
12. P.C.Mishra, “Chemistry of natural products” Vol.II,2011, Alfa publications, New Delhi.
13. S.P. Bhutani, “Amino acids, Peptides and proteins”, Ane books (p) Ltd, Delhi, 2010.

UNIT - I

(18)

Elements of Group Theory:

- 1.1 Introduction – Symmetry elements, Symmetry operations , n-fold Proper axis of symmetry, Centre of Symmetry, Plane of Symmetry, n-fold Improper axis of Symmetry , Group, Rules for forming a Group, Finite Group, Infinite Group, Abelian Group, Cyclic Group, Sub Groups, Group Multiplication Table- Class and Similarity transformation.
- 1.2 Point Group – Method of Assigning Point Group, Matrix Representation Theory – Matrix Representation of Symmetry operation, Reducible , Irreducible Representation
- 1.3 The Great Orthogonality Theorem – Properties of Irreducible Representation – Construction of Character Table for C_{3V} , C_{2V} Point Groups – Explanation of Character Table – Correlation Table.

Unit – II

(18)

Applications of Group Theory:

- 2.1 The Direct Product and its Applications, Applications of Group theory to Spectroscopy – Vanishing of Integrals, Symmetry selection rules for Vibrational, Raman and electronic spectroscopy.
- 2.2 Infra red Spectroscopy – Reduction Formula – Determination of Normal Modes of Vibration and IR activity for H_2O and NH_3 Molecule, Vibrational Raman Spectroscopy for H_2O and NH_3 Molecule, Electronic Spectra of Formaldehyde
- 2.3 Hybridization Schemes of Orbitals (sp^3 , sp^2 , dsp^2 , sp^3d^2), Projection Operator – Symmetry Adapted Linear Combination (SALC) Procedure. Symmetry factoring of secular determinant and its applications to butadiene.

Unit – III

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Ionics:

- 3.1 Transport of ions in solution - Debye - Huckel Onsager theory - Debye - Falkenhagen and Wiens effects - extension to Debye Huckel Onsager theory.
- 3.2 Activity of ions in solutions - Experimental determination - Debye -Huckel limiting law, activity coefficient at higher concentration - Bjerrum model.
- 3.3 Electrode - electrolyte equilibrium - Nernst equation and its limitations - equilibrium electrode potentials - classification of electrodes, concentration cells, liquid junction potentials - Thermodynamic quantities from E.M.F data.
- 3.4 Electrochemical energy - storage systems - primary and secondary batteries - fuel cells.

UNIT- IV

(18)

Electro Kinetic Phenomena and Electrode Kinetics:

- 4.1 Electrical double layer potential – Theory of multiple layers at electrode – Helmholtz, Gouy-Chapmann, Stern, Devanathan models, electrokinetic phenomena – electrophoresis, electroosmosis streaming potential and sedimentation potential, electrocapillary phenomena .
- 4.2 Process at Electrode – Rate of Charge Transfer- Current Density – Butler-Volmer equation – Tafel equation.
- 4.3. Principles of Electro deposition of Metals, Electro chemical corrosion of Metals – Construction and use of Pourbaix and Evans diagrams and Prevention of Corrosion – Electro Chemical oxidation and Reduction

UNIT-V

(18)

Solution Kinetics:

- 5.1 Factors influencing reaction rates in solution - application of Arrhenius equation to solution kinetics, effects of solvents, double sphere and single sphere model and effect of ionic strength - influence of pressure on rates in solution - significance of volume of activation.
- 5.2 Homogeneous catalysis: Acid-Base catalysis - Hammett-Deyrup acidity function - Bronsted relation - Enzyme catalysis - mechanism of single substrate reactions - Michaelis - Menten law - influence of pH and temperature.
- 5.3 Fast reactions: Study of kinetics by stopped flow technique, relaxation methods T and P Jump methods flash photolysis and magnetic resonance methods (NMR & ESR).

REFERENCES:

1. F.A.Cotton, Chemical Application of Group Theory. 2nd Edn. Wiley – Eastern Press,1995.
2. K.V.Raman Group theory and its Application to Chemistry. Tata McGraw –Hill Publishing Company Limited New Delhi,2000.
3. H.Goldstein, Classical Mechanics, Addison – Wesley Publishing company, 1956. L.I.Antropov theoretical electrochemistry, Mir Publishers, Moscow.
4. D.R.Crow, Principles and applications of electrochemistry, 3rd edition Chapman and Hall, London,1985.
5. John Albery, Electrode Kinetics, Clarendon press, oxford, 1975.
6. P.H.Rieger, Electro Chemistry, Chapman Hall, U.S.A., 2010.
7. Peter Atkins and Julio de Paulo – “Atkins physical chemistry” oxford university press- 2010.
8. John O’M Bock ris and Amulya K.N Reddy – “Modern electrochemistry” Ane Book India -2008.
9. Samuel H.Marion Coal F.prupton – “ Principles of Physical chemistry”, Oxford and IBH Publication Pvt.Ltd.

UNIT-I

(18)

NMR Spectroscopy:

- 1.1. Chemical shifts and coupling constants (spin - spin coupling) involving different nuclei (H^1 , P^{31} , C^{13}) interpretation and applications to inorganic compounds. Effect of quadrupolar nuclei (H^2 , B^{10} , B^{11} , N^{14}) on the H^1 NMR spectrum. NMR of paramagnetic molecules - isotopic shifts, contact and pseudocontact interactions - Lanthanide shift reagents - stereochemistry of non - rigid molecules
- 1.2. **ESR Spectroscopy:** Basic principles – presentation of spectra – hyperfine splitting – isotropic and anisotropic hyperfine coupling constants – Mc Connell relation – g value – factors affecting the magnitude of g values – calculation of unpaired electron density on an atom in a delocalized system.
- 1.3. Factors affecting the g values of transition metal ions – dependence of spin-orbit coupling and crystal field effects – zero field splitting and Kramer's degeneracy – effective spins – mixing of states and zero field splitting – line widths in solid state EPR – relaxation and exchange processes – EPR spectra of transition metal complexes – spectrum of bis(salicylaldimine)copper(II) – peroxo complex of cobalt – spin dilution.

UNIT-II

(18)

- 2.1 **Photoelectron spectroscopy :** Basic principles - UPES, XPES and AES – valence and core binding analysis – Koopmans theorem-ESCA and Auger spectroscopy - applications.
- 2.2 **Photochemistry of coordination compounds :** Photochemical reactions of coordination and organo-metallic compounds - photo oxidation, reduction, substitution and photoisomerisation reactions.
- 2.3 **Magnetic properties :** Types of magnetism – dia, para, ferro and antiferro magnetism – magnetic properties of free ions - first and second order Zeeman effects – states $\approx kT$ – states $\ll kT$ – magnetic properties of T terms – temperature independent paramagnetism – anomalous magnetic moment – ferromagnetic and antiferromagnetic exchanges.

UNIT – III

(18)

- 3.1 **Medicinal Bioinorganic Chemistry:** Bioinorganic Chemistry of essentially toxic metals. Lead, Cadmium, Mercury, Chromium. Detoxification by metal chelation.
- 3.2 **Chemotherapy:** Chemotherapy with compounds of certain non-essential elements. Cisplatin – Cancer therapy – cytotoxic compounds of other metals – Gold containing drugs as antirheumatic agents – Lithium in psychopharmacological drugs.
- 3.3 **Radiotherapy:** Radioisotopes of Th, Co, Ra, I₂, Na and Tc.

UNIT – IV

(18)

- 4.1 **Metals at the centre of photosynthesis:** Primary processes – PS – I and II – Charge separation and electron transport – Manganese catalysed oxidation of water to O₂.
- 4.2 Complexes of alkali and alkaline earth metal ions with macrocycles – Poly ethers, spiranes, cryptands – ion channels – ion pumps (K^+ , Na^+ , Ca^{2+}).
- 4.3 **Metal Clusters:** Dinuclear clusters – Structure of Re_2Cl_8 – quantitative MO diagrams for Dinuclear Re and Mo complexes to explain the strength of quadruple bond – polynuclear clusters, polyacids – iso and heteropolyacids of V, Mo and W.

UNIT-V

(18)

- 5.1. **Solid state:** Difference between point group and space group – screw axis – glide plane - symmetry elements – crystal classes – crystal systems – unit cell - Bravais lattices – equivalent positions - relationship between molecular symmetry and crystallographic symmetry – The Concept of reciprocal lattice and its applications – X-ray diffraction by single crystal – rotating crystal and moving film methods – structure factor – systematic absences – determination of space group – Fourier synthesis – heavy atom method – refinement of the structure.
- 5.2. **Neutron diffraction:** Elementary treatment – comparison with X-ray diffraction.
- 5.3. **Electron diffraction:** Basic principles.

REFERENCES:

1. A. Abdul Jameel – “Application of Physical Methods to Inorganic Compounds”, Jan Publications, (2007).
2. A.D.P. Lever, Inorganic Electronic Spectroscopy, 2nd Edition, Elsevier, London, 1984.
3. Nakamoto, Infrared spectra of coordination compounds.
4. P.S. Kalsi – “Spectroscopy of Organic Compounds”, 6st Ed., New Age International Publishers, (2004).
5. H. Kaur – “Spectroscopy”, 3rd Ed., Pragati Prakasan Publications, Meerut, 2006.
6. E.A.V. Ebsworth, W.H. Rankin, Cradock – “Structural Methods in Inorganic Chemistry”, ELBS, 1987.
7. Anthony P. West, solid state Chemistry and its applications, John Wiley, New York, 2000.
- 8 John O’M Bockris and Amulya K.N. reddy K.Maria Gamboa –Aldeco “ Modern electrochemistry 2A” 2nd Edition ., Springer (India) Pvt.Ltd, 2002.

Semester III

CORE – XII

11PCH3412

ORGANIC CHEMISTRY – III (90 Hours) (6 Hrs / Week)

UNIT – I

(18)

1.1 Ultraviolet and Visible Spectroscopy:

Basic principles of electronic transitions - correlation of energy change with electronic transitions. Applications of UV - visible spectroscopy - Woodward – Fieser - Scott rules -applications to conjugated dienes, trienes, polyenes, unsaturated carbonyl compounds, conjugated cyclic ketones and acetophenones - benzene and its substituted derivatives, Stereochemical factors affecting electronic spectra of biphenyl and binaphthyl, cis and trans isomers - angular distortion and cross conjugation, charge transfer spectra.

1.2 Infrared Spectroscopy:

Types of stretching and bending vibrations - characteristics group frequencies – Fermi resonance - organic structure determination. Finger print region, factors affecting IR frequency - identification of functional groups - hydrogen bonding

(intermolecular and intramolecular) - conformational aspects in cyclic 1,2- diols and 1,3-diols trans annular interaction in UV and IR - Determination of reaction rates and mechanisms of reactions employing IR and UV spectroscopy (basic aspects).

UNIT – II (18)

2.1 Proton NMR Spectroscopy:

Chemical and magnetic non-equivalence - chemical shift – Factors influencing δ values - coupling constant -first and second order proton, spin-spin splitting dependence of J on dihedral angle, vicinal and geminal coupling constants. Karplus equation, Long range coupling constants. Influences of stereochemical factors on chemical shift of protons - simplification of complex spectra - double resonance techniques, shift reagents. Chemical spin decoupling of rapid, exchangeable protons (DH, SH, COOH, NH₂.) an elementary treatment of NOE phenomenon - 2D techniques (COSY, NOSEY and ROSY).

2.2 ¹³C NMR Spectroscopy:

Basic principles - FT/NMR/relaxation - broad band decoupling, off- resonance decoupling, α , β and γ -effects of substituents. Calculation of chemical shifts for simple aliphatic and aromatic compounds - conformation and chemical shift correlations - peak assignments. Importance of NOE phenomenon in ¹³C NMR spectroscopy.

UNIT – III (18)

3.1 Mass Spectroscopy:

Basic principles - resolutions - EI and CI methods - base Peaks, isotopic peaks, metastable peaks, parent peaks, determination of molecular formula - recognition of molecular ion peak. FAB fragmentation - general rules. Nitrogen rule – Ring rule - fragmentation pattern - McLafferty rearrangement, importance of metastable peaks.

3.2 Electron Spin Resonance Spectroscopy: Basic principles - hyperfine splitting. Applications to simple organic free radicals.

3.3. Combined spectral problem of organic compounds (UV, IR, NMR (¹H, ¹³ C) and Mass).

UNIT – IV (18)

4.1 Organic Photochemistry:

Fundamental concepts - Jablonski diagram - energy transfer characteristics of photoreaction, photoreduction and photooxidation - photoreactions of ketones and enones - Norrish type I & II reactions. Photochemistry of alkenes, dienes and aromatic compounds. Photosensitisation - photoadditions - Barton reaction - Paterno -Buchi reaction.

4.2 Pericyclic Reactions:

Concerted reactions - stereochemistry - orbital symmetry and correlation diagram - Frontier Molecular Orbital approach - Woodward Hoffman rules - electrocyclic reactions - cycloadditions selection rules, - sigmatropic rearrangements - selection rules with simple examples - 1,3 and 1,5 - hydrogen shifts - Cope and Claisen rearrangement.

UNIT – V (18)

5.1 **Optical Rotatory Dispersion and Circular Dichroism:**

Introduction to theory and terminology. Cotton effects and ORD curves. Axial haloketone rule and its applications - octant rule and its applications. Applications of ORD to determine absolute configuration of simple monocyclic ketones.

5.2 **Alkaloids:**

Structural elucidation and medicinal values of Quinine – Reserpine - Morphine – Ergotamine, Acotinine - Cinchonine and Papaverine. (Synthesis not required).

5.2 **Flavones:**

Synthesis and structural elucidation of flavones and isoflavones. Biosynthesis of flavanoids and related polyphenols.

REFERENCES:

1. Y.R. Sharma, Elementary Organic Chemistry spectroscopy, Principle and chemical applications, S.Chand, 1992.
2. Willam Kemp, organic spectroscopy; ELBS, Macmillan, 1991.
3. P.S. Kalsi, spectroscopy of organic compounds, Niley, 1993.
4. P.M. Silvertein, G.C. Bassler and T.C. Morrill, spectroscopic Identification of organic compounds, 3rd Edition, 1995.
5. C.H. Depuy and O.S. Chapman Molecular Reactions and Photo-Chemistry, Prentice Hall, 1975.
6. B.B. Grill, MR. Willis. Pericyclic reactions, Chapman & Hall 1974.
7. J.R. Dyer, Appliaton of Absorption spectroscopy of organic compounds, Prentice Hall, 2000.
8. I.L. Finar, organic chemistry, Vol. II, 5th Edition ELBS -2010
9. Raj, K. Bansal, Hetrocyclic Chemistry, Synthesis Reactions, and Mechanisms, Wiley, 1990.
10. Pavia, Lampman, Kriz, VyVyan, Spectroscopy, Cengage Learning India Pvt Ltd., New Delhi, 2010.
11. P.S. Kalsi – “organic reactions and their Mechanism”, 3th Ed., (2010), New Age International Publishers Ltd., New Delhi

SEMESTER – IV

CORE-XIV

11PCH4414

PHYSICAL CHEMISTRY – III (90 Hours) (6 Hrs / Week)

UNIT – I

(18)

Classical Thermodynamics:

- 1.1 Thermodynamics of systems of variable composition - partial molar property – partial molar quantities of E, V, H, A, G and S, chemical potential, physical significance of chemical potential, variation of chemical potential with respect to T and P, chemical potential in terms of U and H, partial molar quantities from experimental data – direct method, apparent molar properties, intercepts method and general methods.
- 1.2. Calculation of thermodynamic properties of real gases - fugacity concept, variation of fugacity with T and P – calculation of fugacity of real gases, determination of fugacity – graphical method, equation of state method, determination of fugacity in gas mixtures –Lewis-Randall rule.

- 1.3. Activity of non-electrolytes – definition, activity coefficient, standard states of solvent and solute for liquids and solids, dependence of activity on T and P, experimental determination of activity (solvent and solute) – vapour pressure method, cryoscopic method and EMF method.

UNIT - II (18)

Statistical Mechanics:

- 2.1. Basic Concepts and Classical Statistics – introduction of statistical mechanics, mathematical probability, thermodynamic probability, relation between mathematical probability and thermodynamic probability of a system, Boltzmann-Planck's equation, Phase space, Ensembles – types of ensembles, definition of micro and macro states, different methods of counting macro states, postulates, Ergodic hypothesis, distinguishable and indistinguishable particles, Stirling's approximation
- 2.2. Classical statistics – derivation of Maxwell-Boltzmann statistics and distribution law, partition functions – definition, derivation of translational, rotational, vibrational and electronic partition functions, principle of equi-partition of energy.
- 2.3 Molar partition function and molecular partition function, partition functions and thermodynamic quantities - Internal energy (E), heat capacity (Cv), work function (A), pressure (P), heat content (H), Gibb's free energy(G) and entropy(S), entropy of mono atomic gases (Sackur-Tetrode equation)

UNIT -III (18)

Quantum Statistics:

- 3.1. Quantum statistics – Bose-Einstein and Fermi-Dirac statistics and distribution function, comparison of them with Maxwell-Boltzmann statistics,
- 3.2. Application of B.E.statistics - photon gas and super fluidity of liquid helium, concept of negative Kelvin temperature, application of F.D.statistics - electron gas and thermionic emission.
- 3.3. Heat capacities of solids – Dulong and petit's law, classical theory and its limitations, Einstein's theory and its limitations, Debye's theory and its limitations

UNIT-IV (18)

Irreversible Thermodynamics:

- 4.1. Non-equilibrium thermodynamics – definition, types of irreversibility of a process, postulates, entropy production - entropy production and rate in a chemical reaction, Onsagar relations - linear law, reciprocal relation and applications, stationary-state.
- 4.2 **Phase rule-Three component system:**
Maximum number of phases, maximum number of F, Roozeboom triangle-Types- formation of one pair partially miscible liquids, formation of two pairs of partially liquids, Formation of three pairs of partially miscible liquids.
- 4.3. **Solid liquid systems:**
Ammonium chloride - Ammonium nitrate - Water system, H₂O - Na₂SO₄ - NaCl system, MgCl₂, CaCl₂.H₂O system.

Surface Phenomena:

- 5.1 B.E.T. isotherms - Surface area determination - Heat of adsorption and its determination Adsorption from solution, Gibbs adsorption isotherm - solid - liquid interfaces - wetting and contact angle - solid gas interfaces - soluble and insoluble film.
- 5.2 Surface tension - methods of measuring surface tension - electrical phenomenon at Interfaces, including electro kinetic, micelles and reverse micelles, Solubilisation, Micro - emulsions.
- 5.3 Role of surface in catalysis - semiconductor catalysis, n and p type surfaces - kinetics of surface reactions involving adsorbed species - Langmuir - Hinshelwood mechanism.

REFERENCES:

1. F.W.Sears – Statistical Mechanics 2nd Ed. 1972 Addison Wesley.
2. KKuriacose and Rajaram – Thermodynamics for Students of Chemistry Shoban Lalnagin Chand & Co.Delhi 2002.
3. Gurdeep Raj – Thermodynamics Statistical Thermodynamics & Irreversible Thermodynamics Goel Publishing House, Meerut, 1998.
4. H.W.Zemansky – Heat and Thermodynamics M cGraw Hill, 1975.
5. P.W.Atkins – Physical Chemistry E.L.B.S. 6th Ed.1998.
6. Samuel Glasstone – Textbook of Physical Chemistry 2nd Ed.1981, MacMillan India.
7. K.L.kapour – A text book of physical chemistry Volume -4 S.M.yogan at Machmillaln India press, Chennai -2009.

Semester I

CORE –IV

11PCH1404: P

INORGANIC CHEMISTRY PRACTICAL – I**Qualitative Analysis and Colorimetric Estimation:***Semi-micro Qualitative Analysis**Analysis of two common and two rare earth elements in a given inorganic mixture*

Common: Pb, Cu, Bi, Cd, Zn, Co, Ni, Ca, Ba, Sr

Rare: W, Se, Te, Mo, Ce, Zr, Th, V, Li

Colorimetric Estimation:

Cu, Fe, Mn, Ni, Cr

Semester- I

CORE- V

11PCH1405: P

ORGANIC CHEMISTRY PRACTICAL - I

Organic Mixture Analysis and Chromatographic Techniques;

Separate the following types of mixture and analyse only one of the components present as desired by the Teacher/Examiner

1. Mixture Analysis:

1. Soluble and insoluble
2. Acidic and Neutral
3. Less acidic and neutral
4. Basic and neutral

2) Two Stage Preparation:

- (i.) Acetylsalicylic acid from methylsalicylate
- (ii.) 1, 3, 5 – Tribromobenzene from Aniline
- (iii.) *p*-Nitroaniline from acetanilide
- (iv.) *p*-Bromoaniline from acetanilide
- (v.) Benzilic acid from benzoin
- (vi.) Benzaldehyde to chalcone epoxide via chalcone
- (vii.) Cyclohexanone to caprolactone via cyclohexanone oxime

INORGANIC CHEMISTRY PRACTICAL - II**Volumetry, Gravimetry Estimations and Complex preparation:****Estimation of the following elements by volumetric and gravimetric methods:**

1. Cu (V) Ni (G)
2. Cu (V) Zn (G)
3. Cu (V) Mg (G)
4. Zn (V) Cu (G)
5. Fe (V) Zn (G)
6. Ca (V) Mg (G)

Note: V – Volumetric
G – Gravimetric

PREPARATION:

1. Tetramminecopper(II) sulphate
2. Potassiumtrioxalatochromate (III)
3. Hexathiourealead(II) nitrate
4. Potassiumtrioxalatoaluminate (III)
5. Tristhioureacopper(I) chloride
6. Tristhioureacopper(II) sulphate

Semester II

CORE -X

11PCH2410: P

ORGANIC CHEMISTRY PRACTICAL - II

Organic Estimations and Chromatography Technique:

1) Estimation of the following:

Phenol, Aniline, Ethyl Methyl Ketone, Glucose, Ascorbic Acid (Vit-C).

2) Chromatographic Technique:

1. Thin Layer Chromatography

3) Identification of chromophore / functional groups using UV and IR spectra.

CORE – XIII

Semester III

11PCH3413: P

Examination: 6 Hrs.

II PG PHYSICAL CHEMISTRY PRACTICAL – I

ELECTROCHEMISTRY EXPERIMENTS:

CONDUCTOMETRY:

1. Estimation of mixture of acids.
2. i. Determination pK_a – Ostwald's dilution law.
ii. Determination of solubility product-Kohlrausch's law.
3. Estimation of mixture of halides.
4. Determination of hydrolysis constant (for aniline hydrochloride)
5. i. Saponification of ethyl acetate (Kinetics study).
ii. Determination of critical micelle concentration by conductometric method.

POTENTIOMETRY:

1. Estimation of mixture of acids.
2. Determination of solubility product
 - a. Galvanic cell method.
 - b. Concentration cell method.
3. Estimation of mixture of halides.
4. Determination of $E^{\circ}_{Zn^{2+}/Zn}$ and estimation of Zn^{2+} .
5. Determination of hydrolysis constant (for aniline hydrochloride).

II PG PHYSICAL CHEMISTRY PRACTICAL - II

NON-ELECTROCHEMISTRY EXPERIMENTS:

1. Phase diagram of a binary system (Eutectic formation)
2. Phase diagram of a two-component system forming compound (with congruent melting point).
3. Phase diagram of a three component liquid system (with one partially miscible pair) (Toluene-Water-Acetic acid).
4. Heat of solution of benzoic acid in water.
5. Comparison of strengths of three acids from kinetic study (Iodination of acetone)
6. Rast micro method of determining k_f and molecular weight.
7. Determination of E_a and A (for the hydrolysis of ethyl acetate at different temperatures)
8. Primary salt effect (on the kinetics of reaction between $S_2O_8^{2-}$ and I).
9. Verification of Freundlich adsorption isotherm (Adsorption of oxalic acid on Charcoal).
10. Estimation of KI by partition method.

SEMESTER- III

CORE BASED ELECTIVE - I

11PCH3501

PHARMACEUTICAL CHEMISTRY (90 Hours) (6 Hrs / Week)

UNIT-I

(18)

- 1.1. **Drugs:** Introduction - nature and source of drugs – study of drugs - important terminologies - pharmacology, pharmacy, pharmacodynamics, pharmacophore, metabolites virus, antimetabolites, bacteria, fungi - chemotherapy pharmacopoeia - actinomycetes.
- 1.2. **Causes and symptoms of common diseases:** tuberculosis, asthma, jaundice, leprosy, typhoid, malaria, cholera, classification of drugs –biological, chemical commercial consideration and lay public.
- 1.3. **Indian medicinal plants and trees** – Medicinal properties of Adathoda, tulsi, thoothuvalai, margo and kizhanelli.

UNIT-II

(18)

- 2.1. **Antibiotics:** Definition, classification – properties – therapeutic uses of chloramphenicol, penicillin, streptomycin and tetracycline.
- 2.2. **Sulpha drugs:** mechanism of action of sulpha drugs, sulphanilamide, General properties and drug action. Preparation and uses of sulphadiazine, sulpha pyridine, sulpha thiazole, sulpha furazole.
- 2.3. **Vitamins:** classification - Fat soluble vitamins A, D, E, K and water soluble vitamin B complex and vitamin C - deficiency and symptoms.

UNIT-III

(18)

- 3.1. **Analgesics:** Definition – classification – narcotic and non-narcotic types – morphine and its derivatives. Synthetic analgesics – Pethidines and methadones – preparation, properties and uses.
- 3.2. **Antipyretic Analgesics:** Salicylic acid derivatives, aminophenol derivatives, mechanism of action – uses. Anti-Inflammatory Drugs: Indolyl derivatives – indomethacin – ibuprofen – properties and uses
- 3.3. **Anti-Histamine:** definition – Diphenhydramine and phenothiazines – properties – uses.

UNIT-IV

(18)

- 4.1. **Antiseptics and Disinfectants:** Definition - standardization – use of phenols – dyes – chloramines – organo mercurials – formaldehyde - cationic surface active agents - uses.
- 4.2. **Anaesthetics:** Definition – classification – general volatile anaesthetics – ethers, nitrous oxide, chloroform, trichloro ethane, storage – advantage – disadvantages – intravenous anaesthetics – thiopental sodium, methohexitone – local anaesthetics – cocaine, procaine, benzocaine – uses – advantage - disadvantages
- 4.3. **Cardiovascular drugs:** classification – antiarrhythmic drugs, antihypertensive drugs, synthetic antihypertensive drugs – mode of action and uses.

UNIT-V

(18)

- 5.1. **Cancer and Antineoplastic Drugs:** Definition, causes of cancer, antineoplastic agents, cytotoxic antimetabolites - plant products, hormones.
- 5.2. **Diabetes and Hypoglycemic Drugs:** Types-causes- symptoms – control methods insulin - oral hypoglycemic agents - sulphonyl urea – adverse effects.
- 5.3. **Anticonvulsant agents:** Definition, types, barbiturates, hydantoins, succinimides – acetyl urea derivatives -uses.

REFERENCES:

1. Aleg gringaur Introduction to medicinal chemistry.Sharma Printers Delhi, 2011.
2. Mathew George & Lincy joseph Text book of pharmaceutical chemistry 2009.
3. D.Sriram & P.Yogeshwari Medicinal chemistry second edition-2008.
4. Ashutoshkar Medicinal chemistry V revised and expanded edition, International publishers. 2010.
5. Jayashree Ghose – Text book of Pharmaceutical chemistry, II Edn., 2003.
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7. Pharmaceutical Chemistry, Vol. I and Vol.II, v.n. Rajasekaran Sun publications Chennai. 4th Edn. 2003.
8. Applied Chemistry K.Bagavathi Sundari MJP Publishers Chennai, I Edn., 2006.
9. Medicinal chemistry , V.K.Ahluwalia and madhu chopra, Ane books private Ltd. New Delhi, 1st Edition, 2008 .
10. Pharmacology, Marlin Herbert – Ashton Nany darkson,jones and Bartlett India Pvt.Ltd. 1th Edition, 2010.

SEMESTER – III CORE BASED ELECTIVE – II 11PCH3502
ANALYTICAL METHODS IN CHEMISTRY
(90 Hours) (6 Hrs / Week)

UNIT-I (18)

- 1.1 **Analytical chemistry** - chemical analysis – Advantages and limitations of Chemical methods- types of chemical analysis- Instrumental methods- Advantages and Limitations of Instrumental methods- Analytical methods on the basis of Sample size – Sampling- sampling methods- sampling in different physical states- Sampling statistics- source of error in sampling- dangers during sampling.
- 1.2 **Techniques of Analysis** – Introduction- Classification of analytical techniques- classification of instrumental methods of analysis - factors affecting the choice of analytical methods- interferences- typical separation procedures- sensitivity and detection limits.
- 1.3 **Statistical Analysis of Data:**
Various types of errors – Precision and Accuracy – significant figures, mean value, variance and standard deviation.

UNIT-II (18)

- 2.1 **Solvent extraction:** Principle, types of extractant system- Extraction of liquids – Batch extraction process, continuous extraction process – Extraction by chemically active solvents- Extraction of solids – Drying agents- MgSO₄, anhydrous CaCl₂, anhydrous K₂CO₃, anhydrous CaSO₄ - Distillation theory – Steam distillation- fractional at atmospheric pressure- Vacuum/reduced pressure distillation.
- 2.2 **Recrystallisation** – solvent selection – Handling of flammable solvents – Use of decolourising Carbon – Difficulties in recrystallisation – recrystallisation at very low temperature – semi micro and micro recrystallisation – Drying of recrystallised materials.

UNIT-III (18)

- 3.1 **Fluorimetry:** Fluorescence – mechanism – Fluorimetry – theory – Instrumentation application -comparison of absorption and fluorescence methods, spectrofluorimeters – principle – Instrumentation and applications.
- 3.2 **Turbidimetry and nephelometry:** Theory – Instrumentation and applications.
- 3.3 **Flame photometry and Phosphorimetry** – Principle – instrumentation – working – applications.

UNIT-IV

(18)

- 4.1 **Colorimetry:** principles, laws of colorimetry, instrumentation for visual and photolorimetry, types of photo colorimeters – single beam and double beam-working – advantages - colorimetric estimation of Ni, Cu and Fe.
- 4.2 **Polarography:** Introduction – principle – Ilkovic equation – Instrumentation – working advantages of DME – evaluation of polarographic curves – applications of polarography – pulse polarography.
- 4.3.1 **Thermo analytical methods:** thermo gravimetric analysis – principle – instrumentation – TG curve – factors affecting TGA - applications – Differential thermal analysis –DTA curves – applications – Differential Scanning Calorimetry – Thermometric titrations – principle – applications.

UNIT-V

(18)

- 5.1 **Voltammetry:** Instrumentation, capacitive current, linear potential sweep (dc) voltammetry – cyclic voltammetry, potential step methods – normal pulse, differential pulse and square wave voltammetry, stripping voltammetry – principles, electrodes used for stripping analysis, anodic and cathodic stripping voltammetry, voltammetry applications.
- 5.2 **Amperometry:** Amperometric titrations, principles, titrations with dropping mercury electrode (DME), apparatus, biamperometric titrations, advantages and applications of amperometric titrations.
- 5.3 **Coulometry:** Introduction – coulometric titrations – detection of end points – applications in titrimetric analysis – potentiostatic coulometry – advantages.

REFERENCES:

1. H. Kaur - "Instrumental methods of Chemical Analysis", 6th edition, (2010), Pragati prakasan Publications, Meerut.
2. Willard, Merritt, Dean and Settle – "Instrumental Methods of Analysis", 7th Ed., (1983), CBS Publishers.
3. B.K. Sharma – "Instrumental methods of Analysis", (2000), Goel Publications.
4. S.M. Khopkar, "Basic Concepts of Analytical Chemistry", Revised edition (2006) Wiley Eastern Ltd.,
5. R.A. Day and A.L. Underwood – "Quantitative Analysis", (1999), Prentice-Hall of India Pvt., Ltd., New Delhi.
6. B.S. Furniss, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell – "Vogel's Text book of Practical Organic Chemistry", first Indian reprint, (2004), Pearson Education Publisher.
7. L.Pavia – "Spectroscopy" cengage learning India Pvt. Ltd – 2010.
8. Harald Guther, "NMR Spectroscopy", Wiley india (p) Ltd, 2nd Edn, 2010.

SPECIAL TOPICS IN CHEMISTRY (90 Hours) (6 Hrs / Week)

UNIT-I

(18)

1.1 Retrosynthesis:

Synthons – Synthetic equivalents – Convergent and Linear synthesis – Retrosynthetic tree - Guidelines to a good disconnection – Functional Group Interconversions – One group and two group C-X disconnections – One group C-C disconnections – 1,1 C-C and 1,2 C-C disconnections to synthesise alcohols and carbonyl compounds – Regioselectivity – Michael and Wittig reactions – Use of acetylenes and aliphatic nitro compounds in organic synthesis – Two group C-C disconnections – Diels-Alder reaction – its stereochemical aspects – Robinson annelation.

1.2 Guidelines for solving the problem of chemoselectivity – Umpolung reagents – Protecting groups for alcohols, amines and carbonyl compounds – Deprotection.

UNIT-II

(18)

2.1. Sono Chemistry:

Instrumentation – Physical aspects – Types - Homogeneous liquid phase – Heterogeneous solid-liquid reactions. Synthetic applications – Esterification – Saponification – Hydrolysis/Solvolysis – alkylation – oxidation and reduction reactions – Bouveault reaction.

2.2 Supramolecular Chemistry:

Introduction – molecular forces, molecular recognition - basic concepts of host - guest complexation with examples from ionophore chemistry – non-covalent interactions - molecular receptors for different types of molecules, design and synthesis of co-receptor molecules, triangular, square, rectangular supramolecules.

UNIT-III

(18)

3.1. Nano Scale Materials:

Introduction – classification – Preparation and properties of nano particles – metals, semiconductors, ceramics(oxides, carbides, sulphides) physical methods - vapour deposition methods – chemical methods – sol-gel methods – condensation reactions – controlling particle size and morphology - structure and bonding – chemical properties – size dependent properties – melting point – magnetism – colour – conductivity – arrangements – applications – colour – catalysis – nanoelectronics.

UNIT-IV

(18)

4.1. Carbon Nano Structures:

Introduction – fullerenes C₆₀ and C₈₀ nanostructures – properties and applications. Carbon clusters – carbon nano tubes – fabrication – single and multiwalled nanotubes – preparation of carbon nanotubes by pyrolysis and thermal treatment – growth mechanism of carbon nanotubes – characterization of nano particles using SEM and XRD - electrical properties – mechanical properties – application of carbon nano tubes – field emission and shielding, computers, fuel cells, chemical sensors catalysis – mechanical reinforcement.

4.2. **Nano Composites:** Synthesis procedures - various systems (metal-polymer, metal-ceramics and polymer-ceramics). Characterization – procedures – Applications.

UNIT-V

(18)

5.1. Green Chemistry:

Need for green chemistry – planning of green synthesis – solvent free reactions – microwave assisted synthesis – role of ionic liquids in green chemistry – cleaner technology with super critical fluids, catalytic approach to green chemistry. (Use of zeolites, clays, mesoporous materials) waste water treatment by exploitation and technology at ambient conductors. Remediations method for textile effluents – green chemistry – bio-catalytic reactions.

5.2. **Green reactions:** Aldol condensation, Cannizzaro reaction and Grignard reaction-comparison of the above with classical reactions.

REFERENCES:

1. Nanoscale materials in chemistry, Wiley interscience 2002, Kenneth, J.Klaburde.
2. Stuart Warren organic synthesis, methods and starting materials, the disconnections approach John, Wiley & sons-1992.
3. Futhrhop, Penzlin, organic synthesis concepts, methods and starting materials, Verlag chemie 1983.
4. R.Sanghi & MM srivastva Green chemistry, Narosa 2003.
5. M.M.srivastva & R.Sanghi chemistry for green environment, Narosa 2005.
6. S,Delvin Green chemistry, IVY publication house 2006.
7. C.P.Jr. and F.J.Ownes Introduction to Nano technology John wiley &New jersey 2003.
8. P.S. Kalsi & J.P Kalsi – Bioinorganic, Bioorganic & supra molecular chemistry – New Age International Publishers – 2010.
9. Nanotechnology: Principles and practices Sulabha K. Kulkarni (capital Pvt. Co.)-2002.
10. V.K.Ahluwalia and Renu Aggarwal, Organic synthesis, 2nd edition, Narosa, 2006.
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SEMESTER – IV

CORE BASED ELECTIVE – IV

11PCH4504

INSTRUMENTATION TECHNIQUES

(90 Hours) (6 Hrs / Week)

UNIT-I

(18)

- 1.1 **UV- Visible spectroscopy-** Instrumentation- sources, filters and monochromators, slits, grating, cuvette, radiation detectors and indicators, photoelectric spectrophotometer - types, sources of errors during recording, calibration- presentation of spectral data
- 1.2 **Infrared Spectroscopy:** Dispersive infrared spectrometer- source (Nernst, Globar) monochromator, detector, double-beam spectrophotometer - presentation of spectra- sample preparation techniques for IR, FT-IR- simple diagram of a Fourier transform infrared spectrometer- working mode – advantages.
- 1.3 **Raman spectroscopy:** Instrumentation- source of light, filters, sample holders, spectrograph, detectors, Sample preparation.

UNIT-II

(18)

- 2.1. **Nuclear Magnetic Resonance (NMR):** Instrumentation - magnet, magnetic field sweep, radio frequency source, signal detector and recording system, sample holder, sample probe.
- 2.2. **Electron Spin Resonance (ESR):** Instrumentation - electromagnet, source of micro wave radiation, sample cavity, choice of solvent, crystal detectors and recorder-double resonance spectrometers.
- 2.3. **Mass Spectrometry:** Instrumentation - sample preparation, generation of ions, analyzer, ion collector and measuring system, resolution- representation of mass spectrum – double focusing mass spectrometer.

UNIT-III

(18)

- 3.1. **Conductometry:** Introduction, laws and definitions of conductance, effects of dilution, conductance measurements, conductometric titrations - apparatus, types and advantages.
- 3.2. **Potentiometry:** electrochemical series, reference electrodes – hydrogen electrode, calomel and silver-silver chloride electrode, measurement of pH – glass indicating electrode, potentiometric titrations, variations in potentiometric titrations, its advantages.
- 3.3. **Atomic Absorption Spectroscopy:** Introduction, principle of AAS, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation – application. Atomic Emission spectroscopy – Introduction, origin of spectra, principle of emission spectroscopy, Instrumentation, measurement of light intensity and applications.

UNIT-IV

(18)

- 4.1. **Column Chromatography:** Definition, Types, Principles of column chromatography. Experimental techniques – Adsorption column – Packing of column – Adsorbents – Characteristics of good adsorbent – Solvent developer's – Techniques of separation – Detectors, applications of column chromatography.
- 4.2. **Thin Layer Chromatography:** Principle, types, experimental techniques of TLC, applications of TLC.
- 4.3. **Paper Chromatography:** Principle, types, experimental techniques of Paper chromatography, applications.
- 4.4. **Ion Exchange Chromatography:** Principle, Ion exchanger and its types, experimental techniques of IEC, applications.

UNIT-V

(18)

- 5.1. **Gas Chromatography:** Principle, types (GSC, GLC), Instrumentation of GC, applications of GC. GC-MS: Principle, instrumentations, applications of GC-MS.
- 5.2. **High Performance Liquid Chromatography (HPLC):** Introduction, principle, characteristic features of HPLC, instrumentation, applications of HPLC.
- 5.3. **Exclusion Chromatography:** Principle, Types, Gel chromatography, Experimental techniques of GPC.

5.4 **Electrophoresis:** Introduction, Types of Paper electrophoresis, Techniques of Paper electrophoresis, thin layer electrophoresis, Zone electrophoresis, Electro dialysis, applications of Electrophoresis.

REFERENCES:

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5. R.A. Day and A.L. Underwood – "Quantitative Analysis", (1999), Prentice-Hall of India Pvt., Ltd., New Delhi.
6. B.S. Furniss, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell – "Vogel's Text book of Practical Organic Chemistry", fifth edition ,2009, Pearson Education Publisher.
7. L.Pavia – "Spectroscopy" cengage learning India Pvt. Ltd – 2010.
8. Harald Guther, "NMR Spectroscopy", Wiley india (p) Ltd, 2nd Edn,2010.
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10. Colin N.Banwell – "fundemendals of Molecular structure Spectroscopy " Mc.Grow –Hill publishing company Ltd. 4th edition '1995.