GOVERNMENT DEGREE COLLEGE (AUTONOMOUS). SIDDIPET
Re-Accredited with “A” grade by NAAC
M.Sc. CHEMISTRY SYLLABUS
(Effective from academic year 2016-2017 under CBCS mode)

SEMESTER –I

Paper 1 CH 101 (INORGANIC CHEMISTRY)

IC 01: Symmetry of molecules
IC 02: Bonding in Metal Complexes - I
IC 03: Coordination equilibria
IC 04: Ligational aspects of diatomic molecules

Teaching hours-4/week
Marks-80

IC-01: Symmetry of Molecules: 15 hrs
Concept of Symmetry in Chemistry – Symmetry Operations – Symmetry Elements: Rotational Axis of Symmetry and Types of Rotational Axes, Plane of Symmetry and types of Planes, Improper Rotational Axis of Symmetry , Inversion Center and Identity Element – More about Symmetry Elements – Molecular Point Groups: Definition and Notation of Point Groups, Classification Molecules in to C1, Cs, Ci, Cn, Cnv, Cnh, C∞v, Dn, Dnh, Dnd, D∞h, Sn (n=even), Td, Oh, Ih, Kh Groups. Descent in Symmetry with Substitution – Exercises in Molecular Point Groups – Symmetry and Dipole moment – Symmetry criteria for Optical activity.

IC – 02: Bonding in metal complexes – I: 15 hrs
Crystal Field Theory: Salient features of CFT, d-orbital splitting patterns in regular Octahedral, tetragonally distorted octahedral, Jahn-Tellor theorem , trigonal bipyramidal, trigonal planar, Pentagonal bipyramidal, and linear geometries. Concept of weak field and strong fields. - Calculation of crystal field stabilization energies (CFSE’s) in six and four coordinate complexes. Types of magnetic behaviour – magnetic susceptibility – calculation of magnetic moment from magnetic susceptibility spin only formula -. Quenching of orbital angular momentum – Determination of magnetic moment from Guoy’s method. Applications of magnetic moment data for the determination of oxidation states, bond type and stereochemistry. Spin crossover: High spin, low spin cross over phenomenon in [Fe(Ophen)2(NCS)2] and [Fe(R2NCS2)3]. Spinels.

IC-03: Coordination Equilibria: 15 hrs
Solvation of metal ions- Metal complex formation in solution-Binary metal complexes. Stability constants (types and relationships between them). – Factors influencing the stability constants: (i) Metal ion effects (charge/size, IP, crystal field effect, John-Tellor effect, Pearson theory of hard and soft acids and bases (HSAB), elecronegativity and hardness and softness, symbiosis. (ii) Ligand effects (Basicity , Substituent effect , Steric , Chelate(size and number of chelate rings), Macrocyclic and Cryptate effects- crown ethers , crypton, size match selectivity or concept of hole size, limitations, Macrocycles with pendent groups– Methods used for the determination of
Stability constants (Basic Principles only): pH metric, Spectrophotometric and Polarographic methods.


**IC – 04: Ligational Aspects of Diatomic molecules:** 15 hrs

**Metal Carbonyls:** Carbon monoxide as a ligand – Molecular orbitals of CO - Donor and Acceptor molecular orbitals of CO; Bonding modes of CO- Terminal and Bridging; Evidence for multiple bonding from Bond lengths and Stretching frequencies; 18 Valence electron rule and its application.

**Metal Nitrosyls:** NO as a ligand – Molecular orbitals of NO – Donor and Acceptor components; Bonding modes of NO – Terminal (Linear, Bent) and Bridging; Structural aspects of [IrCl(PPh3)2(CO)(NO)]+ and [RuCl(PPh3)2(NO)2]+. Stereo chemical control of valence in [Co(diars)2(NO)]2+ and [Co(diars)2(NO)(SCN)]+.

**Metal Dinitrogen complexes:** N2 as a ligand – Molecular orbitals of N2; Bonding modes – Terminal and Bridging; Stretching frequencies; Structures of Ru (II) and Os(II) dinitrogen complexes; Chemical fixation of dinitrogen.

**Suggested References:**
Paper-II: CH 102 T (Organic Chemistry)

OC-01: Stereochemistry
OC-02: Reaction mechanism-1
OC-03: Conformational analysis (Acyclic systems)
OC-04: Heterocyclic compounds & Natural products

Teaching hours-4/week  Marks-80
OC-01: Stereochemistry:  15 hrs

Molecular representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions.


Axial, planar and helical chirality: Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, atropisomerism, planar chiral ansa compounds and trans cyclooctene, helically chiral compounds and their configurational nomenclature

Relative and absolute configuration: Determination of configuration by chemical correlation methods.

Racemisation and resolution techniques: Racemisation, resolutions by direct crystallization, diastereoisomer salt formation chiral chromatography and asymmetric transformation.


OC-02: Reaction mechanism-I:

Electrophilic addition to carbon carbon double bond: Stereoselective addition to carbon carbon double bond; anti addition- Bromination and epoxidation followed by ring opening. Syn addition of OsO4 and KMnO4.

Elimination reactions Elimination reactions E2, E1, E1CB mechanisms. Orientation and stereoselectivity in E2 eliminations. Pyrolytic syn elimination and α-elimination, elimination Vs substitution.

Determination of reaction mechanism: Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping and crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

OC-03: Conformational analysis (acyclic systems):

Conformational isomerism: Introduction to the concept of dynamic stereochemistry. Conformational diastereoisomers and conformational enantiomers .Study of conformations in ethane and 1,2-disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane-2, 3-diol amino alcohols and 1,1,2,2-tetrahalobutanes. Klyne-Prelog terminology for conformers and torsion angles

Conformations of unsaturated acyclic compounds: Propylene, 1-Butene, Acetaldehyde Propionaldehyde and Butanone.

Factors affecting the conformational stability and conformational equilibrium: Attractive and repulsive interactions. Use of Physical and Spectral methods in conformational analysis.

Conformational affects on the stability and reactivity of acyclic diastereoisomers: Steric
and stereoelectronic factors - examples. Conformation and reactivity. The Winstein-Holness equation and the Curtin – Hammett principle

OC-4: Heterocyclic compounds & Natural products: 15 hrs

Heterocyclic compounds: Introduction, Nomenclature Synthesis and reactivity of indole, quinoline, isoquinoline, carbazole and acridine

Natural products: Importance of natural products as drugs.


Alkaloids: General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine

References:
1. Stereochemistry of carbon compounds by Ernest L. Eliel and Samuel H. Wilen
2. Stereochemistry of organic compounds- Principles and Applications by D. Nasipuri
8. Advanced Organic Chemistry by Jerry March
9. Mechanism and Structure in Organic Chemistry S. Mukerjee
PC-01: Thermodynamics-I
Thermodynamic relations. Gibbs equations. Maxwell relations.
Chemical potential of ideal gases. Ideal-gas reaction equilibrium—derivation of equilibrium constant. Temperature dependence of equilibrium constant—the van’t Hoff equation.

PC-02: Electrochemistry-I
Concept of ion association—Bjerrum theory of ion association (elementary treatment)—ion association constant—Debye-Hückel-Bjerrum equation.

PC-03: Quantum Chemistry-I
A brief review of Black body radiation—Planck’s concept of quantization—Planck’s equation, average energy of an oscillator (derivation not required), Wave particle duality and uncertain principle—significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schrödinger wave equation.


Particle in a box- one dimensional and three dimensional. Plots of $\psi$ and $\psi^2$-discussion. Degeneracy of energy levels. Calculations using wave functions of the particle in a box-orthogonality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.

**PC-04: Chemical Kinetics- I:**

15hrs


Complex reactions- Opposing reactions, parallel reactions and consecutive reactions (all first order type). Chain reactions-general characteristics, steady state treatment. Example- $\text{H}_2\text{-Br}_2$ reaction. Derivation of rate law.

Effect of structure on reactivity- Linear free energy relationships. Hammett and Taft equations-substituent ($\sigma$ and $\sigma^*$) and reaction constant ($\rho$ and $\rho^*$) with examples. Deviations from Hammett correlations, reasons- Change of mechanism, resonance interaction. Taft four parameter equation. Correlations for nucleophilic reactions. The Swain – Scott equation and the Edward equation. Reactions in solutions: Primary and secondary salt effects.

The reactivity-selectivity principle- Isokinetic temperature -Isoselectivity rule, Intrinsic barrier and Hammond’s postulate.

**References:**

1. Atkin’s Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt. Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan
9. Introduction to Electrochemistry, S. Glasstone
11. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford& IBH
Paper-IV: CH 104 (ANALYTICAL TECHNIQUES and SPECTROSCOPY-I)

ASP 01: Techniques of Chromatography  
ASP 02: NMR spectroscopy-I (1H NMR)  
ASP 03: Rotational and Vibrational spectroscopy  
ASP 04: Electronic spectroscopy

Teaching hours-4/week Marks-80

ASP-01: Techniques of Chromatography:  

i. Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory.

ii. GC: Principle, instrumentation, detectors- TCD, FID, ECD. Derivatisation techniques, PTGC.

iii. HPLC: Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector.


ASP 02: NMR spectroscopy-I (1H NMR):

1H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of 1H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Magnetic resonance imaging (MRI). 1H NMR of organic molecules and metal complexes: ethyl acetate, 2-butanone, mesitylene, paracetamol, aspirin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, [HNi(OPEt3)4]+, [HRh(CN)5] (Rh I=1/2), [Pt(acac)2].

ASP 03: Rotational, Vibrational and Raman spectroscopy:


c) **Raman Spectroscopy**- Classical and Quantum theories of Raman effect. Rotational Raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

**ASP 04:Electronic spectroscopy:**  
**Electronic spectroscopy:** Electronic spectra: Elementary energy levels of molecules—selection rules for electronic spectra; types of electronic transitions in molecules. Chromophores: Conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds, Benzene, mono substituted derivative (Ph-R), di substituted derivative (R-C₆H₄-R’) and substituted benzene derivatives (R-C₆H₄-COR’), Woodward-Fieser rules. Polynuclear aromatic compounds (Biphenyl, stilbene, naphthalene, anthracene, phenanthrene and pyrene). Heterocyclic systems. Absorption spectra of charge transfer complexes. Solvent and structural influences on absorption maxima, stereochemical factors. cis-trans isomers, and cross conjugation. Beer’s law application to mixture analysis and dissociation constant of a weak acid.

**References:**
1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
2. Introduction to Molecular Spectroscopy, G.M. Barrow.
5. Introduction to Spectroscopy, Pavia Lampman Kriz.
6. Pharmaceutical analysis, Watson
7. NMR in Chemistry- A multinuclear introduction, William Kemp.
11. Organic Spectroscopy, LDS Yadav
12. Organic Spectroscopy, Y.R. Sharma
13. Molecular Spectroscopy – Arhuldas
14. Vibrational spectroscopy – D.N. Satyanarayana
Practicals:
Paper CH 151: Inorganic chemistry practicals: 6 hrs/week
I. Calibrations:
(i) Calibration of weights.
(ii) Calibration of pipettes.
(iii) Calibration of standard flasks.
(iv) Calibration of burette.
II. EDTA back-titrations:
(i) Estimation of Ni^{2+}.
(ii) Estimation of Al^{3+}.
III. EDTA substitution titrations:
Estimation of Ca^{2+}.
IV. Redox Titrations
(i) Estimation of Ferrocyanide and Ferricyanide in a mixture
V. Preparation of complexes:
(i). Hexaammine nickel (II) chloride.
(ii). Tris (acetylacetanato) manganese.
(iii). Tris (ethylenediamine) nickel (II) thiosulphate.
(iv). Mercury tetra thiocyanato cobaltate (II).
(v). Chloro pentaammine cobalt (III) chloride
(vi). Tetrammine copper (II) sulphate and estimation of NH_{3} and calculation of % purity.
(vii) One component gravimetric estimations
(i) Estimation of Zn^{2+}
(ii) Estimation of Ba^{2+} (as BaSO_{4})

Paper CH 152 Organic Chemistry Lab course 6 hours/week
Synthesis of the following compounds: p-Bromoacetanilide, p- Bromoaniline, 2,4,6-tribromoaniline, 1,3,5-tribromobenzene, aspirin, tetrahydrocarbazole, 7-hydroxy-4-methyl coumarin, m-dinitrobenzene, m-nitro aniline, hippuric acid, azlactone,anthracene-maleic anhydride adduct, Phthalimide, 2,4-dihydroxyacetophenone

References.
1. Text book of practical organic chemistry, Vogel

Paper 153 Physical Chemistry Lab course: 6 hrs / week
Physical properties:
Data analysis I: Significant figures, Precision and accuracy
Distribution:
Distribution of acetic acid between n-butanol and water
Distribution of iodine between hexanes and water
Chemical kinetics:
Acid-catalyzed hydrolysis of methyl acetate
Peroxydisulphate- I- reaction (overall order)
Oxidation of iodide ion by hydrogen peroxide- iodine clock reaction
Conductometry:
Titration of strong acid vs strong base
Titration of weak acid vs strong base
Determination of cell constant
Determination of dissociation constant of a weak acid

**Potentiometry:**
Titration of strong acid vs strong base
Titration of weak acid vs strong base
Determination of dissociation constant of a weak acid
Determination of single electrode potential

**Polarimetry:**
Determination of specific rotation of sucrose
Acid-catalyzed hydrolysis of sucrose (inversion of sucrose)

**Adsorption and others:**
Adsorption of acetic acid on animal charcoal or silica gel
Determination of critical solution temperature of phenol-water system
Effect of added electrolyte on the CST of phenol-water system
Determination of *molecular weight of a polymer by viscometry.*

**References:**
1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical chemistry: J.B. Yadav
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SEMESTER – II

Paper CH 201 INORGANIC CHEMISTRY
IC 05: Reaction mechanisms of transition metal complexes
IC 06: Bonding in metal complexes-II
IC 07: Metal clusters
IC 08: Biocoordination chemistry

Teaching hours/week-4

IC-05: Reaction mechanisms of transition metal complexes: 15 hrs
Ligand substitution reactions:
Energy profile of a reaction – Transition state or Activated Complex. Types of substitution reactions (SE, SN, SN¹, SN²). Langford and Grey classification – A mechanism, D- Mechanism, Ia, Id, and Intimate mechanism.
Ligand substitution reactions in octahedral complexes:
Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis, Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of SN1CB Mechanism.
Substitution reactions with out Breaking Metal-Ligand bond. Anation reaction

Electron Transfer Reactions (or Oxidation-Reduction Reactions) in Coordination compounds: Mechanism of One-electron Transfer Reactions: Atom (or group) Transfer or Inner Sphere Mechanism, Direct electron Transfer or Outer Sphere Mechanism. Factors affecting direct electron transfer reactions, Cross reactions and Marcus-Hush theory.

IC-06: Bonding in Metal Complexes – II: 15 hrs

IC-07: Metal Clusters: 15 hrs
Carbonyl clusters: Factors favouring Metal-Metal bonding – Classification of Clusters – Low Nulcearity Clusters : M3 and M4 clusters , structural patterns in M3(CO)12 (M=Fe,Ru,Os) and M4(CO)12 (M=Co,Rh,Ir) Clusters. Metal carbonyl scrambling – High Nulcearity clusters M5, M6, M7, M8 and M10 Clusters-, Polyhedral skeletal electron pair theory and Total Electron Count theory – Capping rule – Structural patterns in [Os₈(CO)₁₈]³⁻ , [Rh₆(CO)₁₆] , {Os₇(CO)₂₁} , {Rh₇(CO)₁₆}³⁻, {Os₈(CO)₂₂}²⁻ , {Os₁₀C(CO)₂₄}²⁻ and [Ni₅(CO)₁₂]²⁻.
Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems – Edge sharing Bioctahedra, Face sharing Bioctahedra, Tetragonal prismatic and Trigonal antiprismatic structures -. Structure and bonding in $[\text{Re}_2\text{Cl}_{18}]^{2-}$ and Octahedral halides of $[\text{Mo}_6\text{(Cl)}_8]^{4+}$ and $[\text{Nb}_6\text{(Cl)}_{12}]^{2+}$. Trinuclear halides of Re(III). Hoffman’s Isolobal analogy and its Structural implications. Boranes, carboranes, STYX Rule. Stereo chemical non-rigidity in $[\text{Rh}_4(\text{CO})_{12}]$ and $[\text{Fe}_2(\text{Cp})_2(\text{CO})_4]$.

**IC-08: Bio coordination chemistry:** 15 hrs
Metal ions in Biological systems: Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects. Basic principles in the biological selection of elements. Oxygen transport and storage: Hemoglobin (Hb) and Myoglobin (Mb) primary, secondary, tertiary and quaternary structures and non-covalent bonds present in them. Oxygenation equilibria for Mb and Hb. Factor effecting oxygenation equilibria. Cooperativity and its mechanism. Spin state of iron. Spatial and electronic aspects of dioxygen binding. Allosteric models (T and R states). Role of globin. Transport of NO and CO$_2$. Hemocyanin (Hc) and Hemerythrin (Hr): Introduction-structure of active sites with oxygen and without oxygen. Comparison of Hemerythrin and Hemocyanin with hemoglobin.

Photosynthesis: Structural aspects of Chlorophyll. Photo system I and Photo system II. Vitamin B6 model systems: Forms of vitamin B6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation in presence of metal ions.

**References:**
Paper-II: CH 202 T (Organic Chemistry)

OC-05: Reaction mechanism-II
OC-06: Pericyclic reactions-I
OC-07: Photochemistry
OC-08: Reactive intermediates and molecular rearrangements

Teaching hours/week - 4

Marks - 80

OC-05: Reaction mechanism-II: 15 hrs
Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: SN1(Ar), SN2 (Ar), and benzyne mechanisms; evidence for the structure of benzyne. Von Richter rearrangement. Definition and types of ambident nucleophiles.

Neighbouring group participation: Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. Neighbouring group participation involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl, Cycloalkyl groups, σ and π bonds. Introduction to nonclassical carbocations.

Electrophilic substitution at saturated carbon and single electron transfer reactions. Mechanism of aliphatic electrophilic substitution. SE1, SE2, and SEi. SET mechanism.

OC-06 Pericyclic reactions: 15 hrs.
Introduction. Classification of pericyclic reactions,

Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in 4n and 4n+2 systems.

Cycloaddition reactions: suprafacial and antarafacial additions in 4n and 4n+2 cycloadditions.

Sigmatropic reactions: [i, j] shifts- suprafacial and antarafacial shifts, Cope and Claisen rearrangement reactions.


Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical.

Frontier Molecular Orbital (HOMO-LUMO) approach-concept: Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach.

Conservation of orbital symmetry: (Correlation Diagrams) approach for electrocyclic and cycloadditions & cycloreversions.

OC-07 Photochemistry: 15hrs
Photochemistry of \((n - \pi^*)\) transitions: Excited states of carbonyl compounds, homolytic cleavage of \(\alpha\)- bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane diones.


Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2 diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.

OC-08: Reactive intermediates and Molecular rearrangements: 15 hrs

**Reactive Intermediates:** Generation, detection, structure, stability and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals.


References:
1. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
2. Stereochemistry of organic compounds – Principles and Applications by D Nasipuri
3. The third dimension in organic chemistry, by Alan Bassindale
4. Stereochemistry: Conformation and Mechanism by P S Kalsi
5. Stereochemistry by V M Potapov
6. Advanced Organic Chemistry by Jerry March
7. Mechanism and Structure in Organic Chemistry S. Mukerjee
Paper CH 203 PHYSICAL CHEMISTRY
PC-05: Thermodynamics-II & Statistical Thermodynamics
PC-06: Photochemistry-I
PC-07: Quantum Chemistry-II
PC-08: Solid state chemistry

**Teaching hours/week-4**

**Marks-80**

**PC-05: Thermodynamics-II & Statistical Thermodynamics:** 15 hrs

- Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation

**Statistical Thermodynamics:**

- Partition Functions: Concepts of distribution and probability, Boltzmann distribution law. Interpretation of partition functions - translational, rotational, vibrational and electronic partition functions. Relationship between partition functions and thermodynamic functions (only S & G).

**PC-06: Photochemistry –I:** 15 hrs


**PC-07: Quantum chemistry-II:** 15 hrs

- Cartesian, Polar and spherical polar coordinates and their interrelations.
**Bonding in molecules.** Molecular orbital theory - basic ideas. Construction of MOs by LCAO, H2+ ion. The variation integral for H2+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram. The MO wave function and the energy of H2 molecule MO by LCAO method and Valence bond method (detailed calculations not required) - comparison of MO and VB models.

**PC-08: Solid state chemistry:**

15 Hrs


**Nanoparticles and their applications:**


**References:**

1. Atkin’s Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
11. Molecular Photochemistry, N.J. Turro, Benjamin
16. Principles of the Solid State, H. V. Keer, New Age International
17. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press
18. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
19. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
20. Statistical Thermodynamics, M. C. Gupta, New Age International
21. Quantum Chemistry, D. A. McQuarrie, Prentice Hall
25. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.
Paper-IV: CH 204 (ANALYTICAL TECHNIQUES and SPECTROSCOPY - II)

ASP-05: Electro and thermal analytical Techniques.
ASP-06: NMR - II
ASP-07: Mass Spectroscopy
ASP-08: Photoelectron & ESR spectroscopy

Teaching hours/week - 4
Marks - 80

ASP-05: Electro and thermal Analytical Techniques: 15 hrs

I: Types and Classification of Electro analytical Methods:


b) Brief account of following techniques and their advantages over conventional d.c.polarography.
(i) A.C. polarography
(ii) Square-wave polarography
(iii) Pulse polarography
(iv) Differential pulse polarography


d) Cyclic Voltammetry: Principle, instrumentation, Applications. Cyclic voltammetric study of insecticide parathion.

II: Thermal Analysis: 15 hrs

Thermal techniques - Introduction, types of thermo analytical methods. Thermogravimetry principle and applications of thermogravimetry, differential thermal analysis - principle and applications of DTA. Differential scanning calorimetry. DSC: Principle, and application of DSC.

ASP 06: NMR spectroscopy-II (1H, 19F and 31P NMR): 15 hrs

1H, 19F, 31P and solid state NMR spectroscopy: First order and non first order spectra e.g., AX, AX2, AX3, A2X3, AMX and AB, ABC. Simplification of complex spectra: increased field strength, deuterium exchange, Lanthanide shift reagents and double resonance techniques. Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher’s acid. Nuclear Overhauser enhancement (NOE). Fluxional molecules: bullvalene, C5H5Ti and [η1(C5H5)2Ti η1-(C5H5)2] and [η1C8H8Ru(CO)3].

19F NMR spectroscopy: 19F chemical shifts, coupling constants. Applications of 19F NMR involving coupling with 19F, 1H and 31P: 1,2 dichloro-1,1 difluoro ethane, BrF5, SF4, PF5, ClF3, IF5, CF3CH2OH.

31P NMR spectroscopy: 31P chemical shifts, coupling constants. Applications of 31P NMR involving coupling with 31P, 19F, 1H and 13C: ATP, PPh3PSe, P4S3, H3PO4, H3PO3, H2PO2, HPF5, PF5, PH3, [Rh(PPh3)Cl3] (Rh I=1/2)

Introduction to solid state NMR: Magic angle spinning (MAS). Applications of solid state NMR.

ASP 07: Mass spectrometry: 15 hrs

Origin of mass spectrum, principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule). Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β-
cleavage, McLafferty rearrangement, retro Diels–Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

ASP-08: Photoelectron & ESR spectroscopy: 15 hrs

Photoelectron Spectroscopy

Electron Spin Resonance

References:
2. Organic spectroscopy by William Kemp
3. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W. Johnstone
4. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming
5. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake
7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
9. NMR-A multinuclear introduction by William Kemp
10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
Practicals:

**Paper CH 251: Inorganic chemistry practicals**

I. Analysis of Two component mixtures:
(i). Separation of Ni\(^{2+}\) and Cu\(^{2+}\) in a mixture and estimation of Ni\(^{2+}\) (gravimetric) and Cu\(^{2+}\) (volumetric).
(ii). Separation of Fe\(^{2+}\) and Al\(^{3+}\) in a mixture and estimation of Fe\(^{2+}\) volumetrically and Al\(^{3+}\) gravimetrically.
(iii). Separation of Ag\(^{+}\) and Ca\(^{2+}\) in a mixture and estimation of Ag\(^{+}\) volumetrically and Ca\(^{2+}\) volumetrically

II. Analysis of three component mixtures:
(i). Separation of (Ni\(^{2+}\) and Cu\(^{2+}\)) from Mg\(^{2+}\) in the given mixture and estimation of Mg\(^{2+}\) (Gravi).

III Applied titrimetric analysis
(i) Determination of Iron and calcium in Cement 
(ii) Determination of Calcium in calcium tablets 
(iii) Determination of alkali content in antacid 

IV. Ion exchange methods of analysis:
(i). Determination of capacity of an ion exchange resin. 
(ii). Separation of Zinc and Magnesium on an anion exchange resin and estimation of Mg\(^{2+}\) and Zn\(^{2+}\).

**Suggested Books:** (For both semesters).

**Paper CH 252 Organic Chemistry Lab 6 hours/ week**

**Identification of organic compounds systematic qualitative analysis:**
Physical data BP / MP, Ignition test, solubility classification, Extra elements-N,S & Halogens, (Lassagnine sodium fusion test, Beilstein test) Functional groups tests, Preparation of crystalline derivative and determination of their m.p.s and reference to literature to identify the compounds
A minimum of 8 following compounds to be studied as unknown covering atleast one from each of the solubility classes Glucose, benzoic acid, 2-chloro benzoic Acid, Anisic acid, p-Nitrobenzoic acid; p-Cresol, p-Chlorophenol, β-Naphthol; Aniline, o/m/p-Chloroanilines; N-Methyl aniline/N-Ethylaniline, N,N-Dimethylaniline,Benzoamide, Benzaldehyde, Anisaldehyde, Acetophenone,benzophenone,Ethylbenzoate,methylbenzoate,Nitrobenzene, chlorobenzene, bromobenzene , naphthalene, biphenyl anthracene.
Identification of unknown organic compounds from their IR, UV, 1H nmr and MS: Analysis of recorded spectra of 6 compounds belonging to i) aromatic carboxylic acid ii) alcohols and phenols iii) aldehydes and ketones iv) amides v) esters vi) alkenes and alkynes

References
1. Text book of practical organic chemistry, Vogel

Paper CH 253: Physical Chemistry Lab: 6 hrs/week
Data analysis II: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

Distribution:
1) Distribution of I₂ between hexanes / cyclo hexanes / CCl₄ and aq.KI solution- calculation of equilibrium constant.
2) Study of complex formation between ammonia and metal ion

Chemical Kinetics
1) Stoichiometry of peroxydisulphide- iodide reaction
2) Peroxydisulphide- iodide reaction: order w.r.t [I⁻] by isolation method
3) Peroxydisulphide- iodide reaction: order w.r.t [S₂O₅²⁻] by initial rate method

Conductometry:
1) Titration of a mixture of strong and weak acids vs strong base
2) Determination of the hydrolysis constant of aniline hydrochloride
3) Determination of solubility product

Potentiometry:
1) Titration of Fe²⁺ vs Cr₂O₇²⁻ (redox titration)
2) Titration of Cl⁻ vs Ag⁺ (precipitation titration)
3) Determination of solubility product

Polarimetry:
1) Determination of specific rotation of glucose and fructose
2) Enzyme catalysed inversion of sucrose

Colorimetry:
1) Verification of Beer’s law and calculation of molar absorption coefficient using CuSO₄ and KMnO₄ solutions

pHmetry:
1) Calibration of a pH meter and measurement of pH of different solutions
2) Preparation of phosphate buffers
3) Titration of strong acid vs strong base

References:
1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical Chemistry: J.B. Yadav