DEPARTMENT OF CHEMISTRY,
PALAMURU UNIVERSITY, MAHABUBNAGAR, TELANGANA

Minutes of Meeting

The meeting of board of studies in Chemistry is held on 17-11-2021 at 3 PM in the Department of Chemistry, Palamuru University, Mahabubnagar for the operational syllabi from the academic year 2021-22.

The following members were present:

1.	Prof. K.Girija Managatayaru, Dept.of Chemistry, Palamuru University	Chairperson
2.	Prof. P. Leelavathi, Dept. of Chemistry, Osmania University	Member
3.	Dr. MD. Noorjahan, HoD, Dept. of Chemistry, Palamuru University	Member
4.	Dr. N. Chandrakiran, Asst. Prof, Dept. of Chemistry, Palamuru University	Member
5.	Dr. S. Vijaya Laxmi, Asst.Prof, Dept. of Chemistry, Palamuru University	Member
6.	Dr. K. Rajender Reddy, Sr. Principal Scientist, IICT, Hyd	Member
7.	Dr. K. Padmavathi, Principal, NTRGDC for Women, M BNR	Member
8.	Dr. G. Suresh Kumar, Group Leader, Hetero Drugs Ltd, Hyderabad	Member
9.	Dr. A. Hari Padmashri, Asst.Prof, Dept. of Chemistry, Osmania University	Member
10.	Mr. G. Satyanarayana Goud, Asst. Prof, Dr. BRR GDC, Jadcherla	Member

After the discussion the following resolutions were taken.

Resolutions:

1. The Members of the BOS have thoroughly discussed about the existing syllabus and suggested some changes as per the need of current research and Industrial requirements.
2. It is resolved to introduce revised syllabi in accordance with the requirements of CBCS (A copy of the revised syllabus in CBCS pattern is enclosed)
3. Based on the suggestions given by the BOS members, modifications in the syllabus were enclosed in Annexure-1
4. The proposed syllabus for the subject of chemistry is approved unanimously.

K. Girija Noorjahan Kiranmai (Dr N. Chandra Kiran) A. Padmashri P. Leela

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K. Girija Noorjahan Kiranmai (Dr N. Chandra Kiran) A. Padmashri P. Leela

ANNEXURE-1

Following modifications in the syllabus were approved by BOS memebers

Inorganic Chemistry

Semester-1

CH-101-T

IC-01 Symmetry of Molecules 15 hr

No change in the syllabus

IC-02 Bonding in Metal Complexes-I 15 hr

d-orbital splitting in trigonal bipyramidal and pentagonal bipyramidal geometries are introduced.

IC-03 Coordination Equilibria 15 hr

No change in the syllabus

IC-04 Ligational Aspects of diatomic molecules 15 hr

No change in the syllabus

CH-151P Practicals

Preparation of Tetrammine copper (II) sulphate, Petaammine(chloro)cobalt (III) chloride, Sodiumtrioxalato ferrate(III)complexes are included in preparation of complexes

Semester II

Inorganic Chemistry

CH-201-T

IC-05 Reaction mechanism of transition metal complexes 15 hr

No change in the syllabus

IC-06 Bonding in Metal Complexes-II 15 hr

No change in the syllabus

IC-07 Metal clusters 15 hr

No change in the syllabus

IC-08 Bio coordination Chemistry 15 hr

Oxygen transport and storage: Allosteric model (T & S states), transport of CO_2 are included and abbreviations for Haemoglobin (Hb), Myoglobin (Mb), Hemerythrin (Hr) and Hemocyanin (Hc) are included in the syllabus.

CH-251P Practicals

No change in the syllabus

Organic Chemistry

Semester-1

OC-1 Stereochemistry 15 hr

Molecular representations: Wedge, Fisher, Newman and Saw-horse Formulae, their description and interconversions, molecular symmetry & chirality: symmetry operations and symmetry elements (Cn & Sn) to criteria for Chirality removed (since it is already covered in degree final year). Th rest is remained as it is. Determination of Configuration in aldoximes and ketoximes (as an example Beckman rearrangement is included).

OC-2 Reaction Mechanism-1 15 hr

NO change in the syllabus

OC-3 Reaction Mechanism-II 15 hr

Carbohydrates & Proteins removed completely as this topic already included in the elective paper (biomolecules) and also in UG syllabus.

In place of Carbohydrates & proteins, Reaction Mechanism-II from second semester totally shifted to 1st Semester in continuation with Reaction Mechanism-I.

OC-4 Heterocyclic Compounds 15 hr

No change in the syllabus

Practicals

Demonstration of following techniques is included to the od syllabus

1. Recrystallization
2. Steam Distillation
3. Sublimation

Criteria for determination of Purity of organic molecules M.P, mixed M.P and B.P added.

Semester-II (Organic Chemistry)

OC-5 Conformational analysis-I 15 hr

Conformational analysis (acylic systems) is changed to Conformational analysis-I.
From previous syllabus first para is removed as this topic already covered in the degree syllabus
Use of Physical & Spectral methods in conformational analysis is shifted to last paragraph
conformational effects on the stability and reactivity of diastereomers in cyclic systems were added.
Total syllabus from OC-9 conformational analysis cyclic systems (III rd sem) shifted here (Upto cyclo butane)
*For better understanding of chapters like asymmetric synthesis, pericyclic reactions, molecular rearrangements and carbohydrates we need to have a thorough knowledge of conformational analysis of both cyclic and acyclic compounds without which it is very difficult to teach.
Therefore it is recommended to shift the chapters pertaining to conformational analysis in the later semester(III) to the early semester (I) so that many topics which requires conformational analysis can be perfectly understood.

OC-6 Conformational analysis-II and ORD 15 hr

Reaction Mechanism-II is removed & conformational analysis –II and ORD is introduced. Some topics from OC-09 of III Sem from cycloheptane to quinolizidine is introduced. ORD & CD spectroscopy concept from OC-28 is shifted here, as ORD and CD concepts justify the inclusion here.

OC-7 Reactive intermediates and Molecular rearrangements 15 hr

Wagner-Meerwein, pinacol-Pinacolone and Beckmann rearrangements removed (since already covered in degree syllabus and more over Beckmann rearrangement is discussed in OC-I). The rest is remained as it is.

OC-8 Title Changed (Natural Products-I removed) 15 hr

New Title: Natural Products (Terpenoids & Alkaloids)
No Change in the syllabus

Practicals Sem-II

Title Changed:
Previous one: Identification of Organic compounds and Systematic Qualitative analysis
New Title: Systematic Qualitative analysis and Identification of Organic compounds
Identification of Unknown organic compounds from their IR, UV, ^{1}HNMR & Mass Spectral Data changed to Introduction to structural elucidation of organic compounds by IR, UV, ^{1}HNMR & Mass Spectral Data

Physical Chemistry

Semester-1

PC-01 Thermodynamics-I 15 hr

Concepts of I &II laws of thermodynamics and change of entropy calculations in various processes is removed(since already covered in degree syllabus) and Solutions topic from thermodynamics II is included.

PC-02 Electrochemistry-I 15 hr

No Change in the syllabus.

PC-03 Quantum Chemistry-I 15 hr

Particle in a box topic from Quantum chemistry-II is included here as syllabus in Quantum chemistry –I is comparatively less

PC-04 Chemical Kinetics-I 15 hr

No Change in the syllabus

Practicals

No Change in the syllabus
References were added.

Physical Chemistry
Semester-II

PC-05 Thermodynamics-II 15 hr
Solutions topic from Thermodynamics -II is shifted to Thermodynamics –I and Statistical Thermodynamics topic is included here.

PC-06 Photochemistry-I 15 hr
No Change in the syllabus

PC-07 Quantum Chemistry-II 15hr
Particle in a box topic is removed

PC-08 solid state Chemistry 15hr
Magnetic properties of solids topic is removed (since already covered in degree syllabus) and Nanoparticles and their applications topic is introduced here.

Practicals
In distribution experiment CCl_4 is replaced by hexanes/cyclohexanes, in pH metry titration of strong acid vs strong base is included and removed "solutions" experiment.
References were added.

Paper-IV

Semester-1

ASP-01 Techniques of Chromatography 15hr
No Change in the syllabus

ASP-02 NMR Spectroscopy-1 (^{1}HNMR) 15hr
No Change in the syllabus

ASP-03 Rotational & Vibrational Spectroscopy 15hr
No Change in the syllabus

ASP04 Electronic Spectroscopy 15hr
No Change in the syllabus

Semester-II

ASP-05 Electro and thermal Analytical Techniques 15hr
Conductometry and Potentiometry removed from the syllabus as they already present in the Practicals, in place of these two topics we incorporated thermal analysis.

ASP-06 NMR Spectroscopy-II 15hr
No Change in the syllabus

ASP-07 Mass Spectrometry 15hr
No Change in the syllabus

ASP-08 Photoelectron & ESR spectroscopy 15hr
No Change in the syllabus

DEPARTMENT OF CHEMISTRY, PALAMURU UNIVERSTY

M.Sc. Chemistry I &II Semester (CBCS) Syllabus

(Effective from academic year 2021-2022)

[UNDER RESTRUCTURED CBCS Scheme]

(Approved in the P.G. BOS meeting held on -11-2021)

Semester I

Theory	Hrs/week	Internal assessment*	Semester exam	Total	Credits
CH101T	4	20 marks	80 marks	100 marks	4
CH102T	4	20 marks	80 marks	100 marks	4
CH103T	4	20 marks	80 marks	100 marks	4
CH104T	4	20 marks	80 marks	100 marks	4
Lab					
CH151P (IC)	6			50 marks	2
CH152P (OC)	6			50 marks	2
CH153P (PC)	6			50 marks	2
Total				**550 marks**	**22**

Semester II

Theory	Hrs/week	Internal assessment*	Semester exam	Total	Credits
CH201T	4	20 marks	80 marks	100 marks	4
CH202T	4	20 marks	80 marks	100 marks	4
CH203T	4	20 marks	80 marks	100 marks	4
CH204T	4	20 marks	80 marks	100 marks	4
Lab					
CH 251P (IC)	6			50 marks	2
CH252P (OC)	6			50 marks	2
CH253P (PC)	6			50 marks	2
Total				**550 marks**	**22**

*** 15 marks for the written test (Objective type) and 5 marks for the Assignment**

Lab (Practical's) are conducted in two batches (Batch-I & II) with a minimum of 15 students / Batch

M.Sc. CHEMISTRY (CBCS) SYLLABUS
(Effective from the academic year 2021-2022)

SEMESTER –I

Paper-I: CH 101T (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 : **15hrs**

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 C_1, C_s , C_i , C_n ,C_{nv} , C_{nh} ,$C_{\infty v}$, D_n , D_{nh} , D_{nd} ,$D_{\infty h}$, S_n (n=even), T ,T_h , T_d , O , O_h , I, I_h , K_h Groups. Descent in Symmetry with Substitution – Exercises in Molecular Point Groups – Symmetry and Dipolemoment – Symmetry criteria for Optical activity.

IC – 02: Bonding in metal complexes – I: **15hrs**

Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular Octahedral, tetrahedral, Jahn-Tellar theorem- tetragonally distorted octahedral, square planar, trigonal planar, Trigonal bipyramidal, Pentagonal bipyramidal and linear geometries. Factors influencing the magnitude of crystal field splitting in octahedral complexes nature of metal ions, nature of ligands, geometry. 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.

IC-03: Coordination Equilibria: **15hrs**

Solvation of metal ions- Binary complexes: Formation of binary Metal Complexes and their stability – types of Stability Constants – relation between them- trends in Step-wise Stability Constants (Factors causing decrease and increase in Step-wise Stability) – Factors influencing the stability constants :(i) Ligand effects: Basicity, Substituent, Steric, Chelate(size and number of chelate rings), Macrocyclic and Cryptate effects- (ii) Metal ion effects: Ionic potential, Effective Nuclear charge and Atomic Number (Irving-William's Order, geometry of Metal ion and Ligand) – Chelate effect and its Thermodynamic origin – Jahn-Tellar effect on Stability constants of Metal complexes – Pearson's Theory of Hard and Soft Acids and Bases (HSAB), Applications of HSAB, Electronegetivity Vs Hardness and Softness. Symbiosis – Methods used for the determination of Stability constants (Basic Principles only): pH metric, Spectrophotometric and Polarographic methods.

Ternary Metal Complexes – definition – Formation of ternary metal complexes – Step- wise and simultaneous equilibria with simple examples.

IC- 04: Ligational Aspects of Diatomic molecules: 15hrs

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 $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$.
Stereo chemical control of valence in $[Co(diars)_2(NO)]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$.

Metal Dinitrogen complexes: - N_2 as aligand – Molecular orbitals of N_2; Bonding modes –Terminal and Bridging; Stretching frequencies; Structures of Ru (II) and Mo (0) dinitrogen complexes; Chemical fixation of dinitrogen.

Suggested References:

1. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London(2000).
2. Molecular Symmetry and Group Theory, Robert L.Carter, John Wiley & Son (1998).
3. Symmetry and Spectroscopy of Molecules. K.Veera Reddy, New Age International (P) Limited (1999).
4. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann,6 th Edition, Wiley Interscience, N.Y (1999
5. Inorganic Chemistry, J.E.Huheey, K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
6. Homogeneous Catalysis by Metal complexes Vol I, M M Taqui Khan and A E Martell, Academic Press NY (1974).
7. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).

Paper-II: CH 102 T (ORGANIC CHEMISTRY)

OC-01: Stereochemistry
OC-02: Reaction mechanism-I
OC-03: Reaction mechanism-II
OC-04: Heterocyclic compounds

Teaching Hours = 4/week **Marks= 80**

OC-01: Stereochemistry **15hrs**

Desymmetrization. Axial, planar and helical chirality, Configurational nomenclature, Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, atropisomerism. Planar chirality: ansa compounds and trans- cyclooctene. Helically chiral compounds

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

Racemisation, racemates and resolution techniques: Resolutions by direct crystallization, diastereoisomer salt formation, chiral chromatography and asymmetric transformation. **Determination of configuration in *E,Z*-isomers:** Spectral and Chemical methods of configuration determination of *E,Z* -isomers. Determination of configuration in aldoximes and ketoximes using Beckman rearrangement.

OC-02: Reaction mechanism-I **15hrs**

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 OsO_4 and $KMnO_4$

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

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

OC-03: Reaction mechanism-II **15hrs**

Nucleophilic Aromatic substitution reactions: Aromatic Nucleophilic substitution: $S_N1(Ar)$, S_N2 (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 sustitution. S_E1, S_E2, and S_Ei. SET mechanism.

OC-4: Heterocyclic compounds **15hrs**

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms. Synthesis and reactivity of indole, benzofuran, benzothiophene, quinoline, isoquinoline, coumarin, chromone, carbazole and acridine.

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
3. Heterocyclic Chemistry, T.L. Gilchrist, Longman UK Ltd, London (1985).
4. Benzofurans A. Mustafa, Wiley-Interscience, New York (1974).
5. Heterocyclic Chemistry, 3rd Edn J.A.Joule, K.Mills and G..F.Smith, Stanley Thornes Ltd,UK,(1998)
6. The Chemistry of Indole, R.J. Sunderberg, Academic Press, New York (1970).
7. An introduction to the chemistry of heterocyclic compounds, 2nd Edn. R. M. Acheson, Inter science Publishers, New York, 1967.
8. Advanced Organic Chemistry by Jerry March
9. Mechanism and Structure in Organic Chemistry S. Mukerjee
10. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes.
11. Organic Chemistry by Graham Solomous and Craig Fryhle.
12. Organic Chemistry by RT Morrison and RN Boyd.
13. Organic Chemistry, Vol. 2 by I.L. Finar.
14. Organic Chemistry: Structure and Reactivity by Seyhan Ege.

Paper-III: CH 103 T(PHYSICAL CHEMISTRY)

PC-01: Thermodynamics-I
PC-02: Electrochemistry-I
PC-03: Quantum Chemistry-I
PC-04: Chemical Kinetics-I

Teaching Hours = 4/week **Marks= 80**

15hrs

PC-01: Thermodynamics-I

Concept of entropy. Entropy as a function of V and T. Entropy as a function of P and T. Entropy change in isolated systems- Clausius inequality. Entropy change as criterion for spontaneity and equilibrium. Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies and entropy changes of chemical reactions. Helmholtz and Gibbs free energies (A and G). A and G as a criteria for equilibrium and spontaneity. Physical significance of A and G. Driving force for chemical reactions- relative signs of ΔH and ΔS.
Thermodynamic relations. Gibbs equations. Maxwell relations. Temperature dependence of G. Gibbs- Helmholtz equation. Pressure dependence of G.
Chemical potential: Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibium. Clapeyron equation and Clausius-Clapeyron equation .
Conditions for equilibrium in a closed system. Chemical potential of ideal gases. Ideal-gas reaction equlibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.
Solutions: Specifiying the Solution composition. Partial molar poperties-significance. Relation between solution volume and partial molar volume. Measurement of partial molar volumes- slope and intercept methods. The chemical potential. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance.

15hrs

PC-02: Electrochemistry- I

Electrochemical Cells : Derivation of Nernst equation – problems. Chemical and concentration cells (with and without transference). Liquid junction potential – derivation of the expression for LJP – its determination and elimination. Applications of EMF measurements : Solubility product, potentiometric titrations, determination of transport numbers, equilibrium constant measurements. Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration overpotential.
Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient. Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law (derivation not required). Calculation of mean ionic activity coefficient. Limitations of Debye-Huckel theory. Extended Debye-Huckel law.
Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations.
Concept of ion association – Bjerrum theory of ion association (elementary treatment) - ion association constant – Debye-Huckel-Bjerrum equation.

PC-03: Quantum Chemistry- I **15hrs**

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 Schroedinger wave equation.

Operators-operator algebra. Commutation of operators, linear operators.Complex functions. Hermitian operators. Operators and . Eigenfunctions and eigenvalues. Degeneracy.

Linear combination of eigenfunctions of an operator. Well behaved functions. Normalized and orthogonal functions.

Postulates of quantum mechanics. Physical interpretation of wave function. Observables and operators. Measurability of operators. Average values of observables. The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation..

Theorems of quantum mechanics. Real nature of the eigen values of a Hermitian operator- significance. Orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality. Expansion of a function in terms of eigenvalues. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

Particle in a box- one dimensional and three dimensional. Plots of Ψ and Ψ^2-discussion.

Degeneracy of energy levels. Comparison of classical and quantum mechanical particles.

Calculations using wave functions of the particle in a box-orthoganality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.

PC-04: Chemical Kinetics- I **15hrs**

Theories of reaction rates : Collision theory, steric factor. Tranition state theory. Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of transition state theory. Activtion parameters and their significance. The Eyring equation. Unimolecular reactions and Lindamann's theory.

Complex reactions- Opposing reactions, parallel reactions and consecutive reactions(all first order type). Chain reactions-general characteristics, steady state treatment. Example- H_2-Br_2 reaction. Derivation of rate law.

Effect of structure on reactivity- Linear free energy relationships. Hammett and Taft equations-substituent (σ and σ^*)and reaction constant (ρ and ρ^*)with examples. Deviations from Hammett correlations. reasons- Change of mechanism, resonance interaction. Taft four parameter equation. Correlations for nucleophillic reactions. The Swain – Scott equation and the Edward equation.

The reactivity-selectivity principle and the isoselectivty rule. The Hammond's postulate.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
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
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Chemical Kinetics, K.J. Laidler, McGraw Hill
8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan
9. Introduction to Electrochemistry, S. Glasstone
10. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
11. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford& IBH
12. The Physical Basis of Organic Chemistry by Howard Maskill, Oxford University Press (New York)
13. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
14. Physical Organic Chemistry, N. S. Isaacs, ELBS

Paper-IV: CH 104 T (ANALYTICAL TECHNIQUES and SPECTROSCOPY- I)

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

Teaching Hours = 4/week **Marks= 80**

ASP-01: Techniques of Chromatography 15hrs

Introduction to Chromatography: 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.

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

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

Applications: Methods of quantitation for GC and HPLC: GC analysis of hydrocarbons in a mixture, GC assay of methyl testosterone in tablets, atropine in eye drops. HPLC assay of paracetamol and asprin in tablets.

ASP 02: NMR spectroscopy-I (^{1}H NMR) 15hrs

^{1}H 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, geminal and long range, Coupling constants and factors affecting coupling constants. Applications of ^{1}H 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).

^{1}H NMR of organic molecules and metal complexes: ethyl acetate, 2-butanone, mesitylene, paracetamol, asprin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, $[HNi(OPEt_3)_4]^+$, $[HRh(CN)_5]$ Rh I=1/2, $[Pt(acac)_2]$.

ASP 03: Rotational, Vibrational and Raman spectroscopy **15hrs**

a). Microwave Spectroscopy: Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy levels. Selection rules (derivation not required). Calculation of bond lengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer.

b). Vibrational Spectroscopy: Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation force constant from vibrational frequency. Anharmonic nature of vibrations. Fundamental bands, overtones and hot bands, Fermi Resonance. Vibration-rotation spectra diatomic molecules. Vibrations of poly atomic molecules. Normal modes of vibration, concept of group frequencies. Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding. Isotopic effect on group frequency. IR spectra of metal coordinated NO_3^-, SO_4^{2-} and CO_3^{2-} ions.

c). Raman Spectroscopy: Quantum theory of Raman effect, Rotational Raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Ramanspectra.

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 congugated dienes, trienes and polyenes, unsaturated carbonyl compounds, benzene, monosubstituted derivative (Ph-R), di substituted derivative (R-C_6H_4-R') and substituted benzenederivatives (R-C_6H_4-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.
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer.
4. Biochemistry: Hames and Hooper.
5. Introduction to Spectroscopy, Pavia Lampman Kriz.
6. Pharmaceutical analysis, Watson
7. NMR in Chemistry- A multinuclear introduction, William Kemp.
8. Organic Spectroscopy, William Kemp.
9. Spectroscopy of organic compounds, P.S. Kalsi.
10. Structural methods n Inorganic chemistry, E.A.V Ebsworth.

Paper CH 151P: 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. Preparation of complexes:
(i). Hexaammine nickel(II) chloride.
(ii). Tris(acetylacetanato)manganese.
(iii). Tris(ethylenediamine)nickel(II) thiosulphate.
(iv). Mercury tetrathiocyanatocobaltate (II).
(i). Tetramminecopper (II) sulphate
(ii). Pentaammine(chloro)cobalt(III) chloride
(iii). Sodium trioxalato ferrate(III)

Paper CH 152P Organic Chemistry Lab course : 6 hrs / week

Demonstration of following Purification techniques

1. Recrystallization
2. Steam distillation
3. Sublimation

Criteria for detection of purity of Organic molecules

Melting point, mixed melting points, boiling points

Synthesis of the following compounds: p-Bromoacetanilide (using Ceric ammonium nitrate and KBr), p- Bromoaniline, 2,4,6- tribromoaniline, 1,3,5-tribromobenzene, 1,2,3,4-tetrahydrocarbazole, 7-hydroxy-4-methylcoumarin, m-dinitrobenzene, m-nitroaniline, hippuricacid, azlactone, anthracene-maleicanhydride adduct, phthalimide, 2,4-dihydroxyacetophenone and dihydropyrimidinone (using Ethylacetoacetate, Benzaldehyde and Urea).

References.

1. Text book of practical organic chemistry,Vogel
2. Text book of practical organic chemistry, Mann and Saunders.

Paper 153P Physical Chemistry Lab course : 6 hrs / week

Physical properties: Determination of density, surface tension and viscosity of liquids

Distribution:

Distribution of acetic acid between n-butanol and water

Distribution of iodine between Cyclohexane 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

References:

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical chemistr: J.B.Yadav
6. Vogel Text book of Quantitative Analysis, 6th edition, Pearson education Ltd. 2002.

SEMESTER –II

Paper-I: CH 201T (INORGANIC CHEMISTRY)

IC 05: Reaction mechanisms of transition metal complexes

IC 06: Bonding in metal complexes-II

IC 07: Metal clusters

IC 08: Bio coordination chemistry

Marks= 80

Teaching Hours = 4/week

15hrs

IC-05: Reaction mechanisms of transition metal complexes:

Ligand substitution reactions:

Energy profile of a reaction – Transition state or Activated Complex. Types of substitution reactions (SE,SN,SN^1, SN^2).

Ligand substitution reactions in octahedral complexes:

Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis , Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of SN^1CB Mechanism.

Annation reactions.

Substitution reactions without Breaking Metal-Ligand bond.

Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Grienberg's Polarization theory and π - bonding theory – Applications of Trans-effect in synthesis of Pt (II) complexes.

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, Marcus –Hush theory.

15hrs

IC-06: Bonding in Metal Complexes – II:

Free ion terms and Energy levels: Configurations,Terms,States and Microstates – Formula for the calculation of Microstates p^n and d^n configurations – L-S (Russel-Saunders) coupling scheme – j-j coupling scheme – Determination of terms for various p^n and d^n configurations of metal ins. Hole formalism – Energy ordering of terms (Hund's rules) Inter – electronrepulsion Parameters (Racah parameters) – Spin-Orbital coupling parameters. Effect of weakcubic crystal fields on S, P, D and F terms- Orgel Diagrams.

15hrs

IC-07: Metal Clusters:

Carbonyl clusters: Factors favouring Metal-Metal bonding – Classification of Clusters – Low Nuclearity Clusters : M_3 and M_4 clusters , structural patterns in $M_3(CO)_{12}$ (M=Fe,Ru,Os) and $M_4(CO)_{12}$ (M=Co,Rh,Ir) Clusters-. Metal carbonyl scrambling – High Nuclearity clusters M_5,M_6,M_7,M_8 and M_{10} Clusters-, Polyhedral skeletal electron pair theory and Total Electron Count theory – Wades rules – Capping rule – Structural patterns in $[Os_6(CO)_{18}]^{2-}$, $[Rh_6(CO)_{16}]$, $[Os_7(CO)_{21}]$, $[Rh_7(CO)_{16}]^{3-}$, $[Os_8(CO)_{22}]^{2-}$, $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_5(CO)_{12}]^{2-}$.

Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems – Edgesharing Bioctahedra,Face sharing Bioctahedra, Tetragonal prismatic and Trigonal antiprismaticstructures -, Structure and bonding in $[Re_2Cl_8]^{2-}$ and Octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$. Trinuclear halides of Re(III).Hoffman's Isolobal analogy and its Structural Implications.

15hrs

C-08: Bio Coordination Chemistry:

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): Geometric, electronic and magnetic aspects of Dioxygen binding, Oxygen adsorption isotherms and Co-operativity in Hemoglobin and its physiological significance, Allosteric model (T & S states) Role of globin chain, Transport of CO_2. Hemerythrin(Hr) and Hemocyanin(Hc): Structure of deoxy forms, oxygen binding, Geometric, electronic and magnetic aspects. Comparison of Hemerythrin and Hemocyanin with Hemoglobin.

Photosynthesis: Structural aspects of Chlorophyll. Photosystem I and Photosystem II. Vitamin B_6 model systems: Forms of vitamin B_6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation in presence of metal ions.

References:

1. Inorganic Reaction Mechanisms. M.L.Tobe and John Burgess, Addison Wesley Longman (1999).
2. Metal ions in Reaction Mechanisms. K.Veera Reddy. Golgotia Publications (P) Ltd
3. Mechanisms of Reactions in Transition Metal Sites. Richard A Henderson, OxfordScience Publications, London (1993).
4. Inorganic Reaction Mechanisms, F.Basolo and R.G.Pearson, New York (1967).
5. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6 Th Edition, Wiley Interscience, N.Y (1999
6. Inorganic Chemistry, J.E.Huheey , K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
7. Inorganic Biochemistry Edited by G.L.Eichorn, Volume 1 Elsevier (1982).
8. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams(Eds), VCH, NY (1990).
9. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
10. Bioinorganic Chemistry, I.Bertini, H.B.Gray, S.J.Lippard and S.J.Valentine, Viva Low-Priced Student Edition, New Delhi (1998).
    a. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W.Kain and B.Schwederski, John Wiley and Sons, NY (1999).
11. Bioorganic Chemistry – Dugas.

Paper-II: CH 202T (ORGANIC CHEMISTRY)

OC-05: Conformational analysis -I
OC-06: Conformational analysis –II and ORD
OC-07: Reactive intermediates and Molecular rearrangements.
OC-08: Natural products (Terpenoids and Alkaloids).

Marks= 80

Teaching Hours = 4/week

15hrs

OC-05: Conformational analysis - I

Conformational diastereoisomers and conformational enantiomers -. Factors affecting the conformational stability and conformational equilibrium – attractive and repulsive interactions. Study of conformations in 1-butene, acetaldehyde, propionaldehyde and butanone. Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2- halocyclohexanones, cyclopentane, cyclobutane. Conformational effects on the stability and reactivity of diastereomers in cyclic molecules and acyclic molecules-steric and stereoelectronic factors examples. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. stereochemistry of addition to the carbonyl group in a rigid cyclohexanone ring. Use of physical and spectral methods in conformational analysis.

15hrs

OC-06: Conformational analysis – II and ORD

Study of conformations in cycloheptane and cyclooctane. Stereo chemistry of bicyclo[3,3,0]octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and cotton effect. Plain curves and anomalous curves. empirical and semiempirical rules. The axial haloketone rule, the octant rule, helicity rule. Exciton chirality method, Exciton coupling between identical chromophores. Benzene sector and chirality rule. Application of the rules to the study of absolute configuration and conformations of organic molecules.

15hrs

OC-07: Reactive intermediates and Molecular rearrangements

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

Molecular rearrangements: Definition and classification. Molecular rearrangements involving 1) electron deficient carbon: Allylic and Wolf rearrangements. 2) electron deficient Nitrogen: Hofmann, Lossen, Curtius and Schmidt 3) electron deficient Oxygen: Baeyer- Villiger oxidation. 4) Base catalysed rearrangements: Benzilic acid, Favorski , Transannular , Sommlett-Hauser and Smiles rearrangement

15hrs

OC-08: Natural products (Terpenoids and Alkaloids)

Importance of natural products as drugs, Isolation of natural products by steam distillation, solvent extraction and chemical methods. General methods in the structure determination of terpenes.Isoprene rule. Structure determination and synthesis of α-terpeniol and camphor. Biogenesis of monoterpenes. Structure determination and synthesis of β-carotene.General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine and quinine.

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. Optical rotatory dispersion by C Djerassi
7. Optical rotatory dispersion and circular dichroism by P Crabbe
8. Advanced Organic Chemistry by Jerry March
9. Mechanism and Structure in Organic Chemistry S. Mukerjee
10. Organic chemistry Vol.I and II by I.L.Finar
11. Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D..Ollis
12. Organic Chemistry, Vol. 2 by I.L. Finar.
13. Chemistry of Natural Products by Bhat, Nagasampagi and Siva Kumar.
14. Alkaloids by K.W. Bentley.
15. Steroids and Terpenoids by Bentle.

Paper-III: CH 203T (PHYSICAL CHEMISTRY)

PC-05: Thermodynamics-II & Statistical Thermodynamics
PC-06: Photochemistry-I
PC-07: Quantum Chemistry-II
PC-08: Solid state chemistry

Marks= 80

Teaching Hours = 4/week

15hrs

PC-05:Thermodynamics-II & Statistical Thermodynamics

Ideal solutions. Thermodynamic properties of ideal solutions. Mixing quantities. Vapour pressure-Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.

Nonideal systems. Concept of fugacity, fugacity coefficeient. Determination of fugacity. Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non ideal solutions. Determination of activity coefficients from vapour pressure measurements. Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation.

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).

15hrs

PC-06:Photochemistry –I

Electronic transitions in molecules. The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured lifetimes. Quantum yield and its determination. Actinomety-ferrioxalate and uranyl oxalate actinometers-problems.

Derivation of fluorescence and phosphorescence quantum yields. E-type delayed fluorescence- evaluation of triplet energy splitting(ΔEST). Photophysical processes-photophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems, State diagrams, Photochemical primary processes. Types of photochemical reactions- electron transfer, photodissociation, addition, abstraction, oxidation and isomerization reactions with examples. Effect of light intensity on the rates of photochemical reactions. Photosensitization. Quenching-Stern Volmer equation. Experimental set up of a photochemical reaction. Introduction to fast reactions- Principle of flash photolysis.

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

Cartesian, Polar and spherical polar coordinates and their interrelations.

Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour plots and boundary diagrams.

Many electron systems. Approximate methods. The variation method-variation theorem and

its proof. Trial variation function and variation integral. Examples of variational calculations. Paricle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant..

Bonding in molecules. Molecular orbital theory-basic ideas. Construction of MOs by LCAO , H_2^+ ion. The variation an integral for H_2^+ 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 and VB wave functions for H_2 molecule and their comparison.

15hrs

PC-08: Solid state chemistry

Electronic properties of metals, insulators and semi conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semiconductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi conductors. Photo conductivity and photovoltaic effect-p-n junctions.

Superconductivity. Occurrence of superconductivity. Destruction of superconductivity by magnetic fields-Meisner effect. Types of superconductors. Theories of super conductivity-BCS theory.

High temperature superconductors. Structure of defect perovskites. High T_c superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_{7-x}$. Preparation of 1-2-3 materials. Origin of high T_c superconductivity.

Nanoparticles and their applications: Introduction to nanoparticles. Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. One dimensional systems, carbon nano tubes, preparation of nanoparticles –top down and bottom up methods. Preparation of nanomaterials- – sol gel methods, and chemical vapour deposition method; thermolysis. Characterization of nanoparticles –experimental methods – powder X-ray diffraction, transmission electron microscopy (TEM),and atomic force microscopy (AFM) (detailed theory and instrumentation are not required).Optical properties of nanoparticles. Applications of nanoparticles.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
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
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
9. Solid state Chemistry and its aplications, A.R. West, Plenum.
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
11. Molecular Photochemistry, N.J. Turro, Benjamin
12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
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
22. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
23. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press
24. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum
25. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.
26. The physics and chemistry of solids by Stephen Elliott, Wiley Publishers.
27. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.

Paper-IV: CH 204 T(ANALYTICAL TECHNIQUES and SPECTROSCOPY - II)

ASP-05: Electro and Thermal Analytical Techniques.

ASP-06: NMR spectroscopy-II (^{1}H, ^{19}F and ^{31}P NMR)

ASP-07: Mass spectrometry

ASP-08: Photoelectron & ESR spectroscopy

Marks= 80

Teaching Hours = 4/week

15 hrs

ASP-05: Electro and Thermal Analytical Techniques

1. Types and Classification of Electro analytical Methods

a) **D.C Polarography :** Dropping mercury electrode- Instrumentation-polarogram. Types of Currents : Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents : Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

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

c) Amperometric titrations :Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances.

d) Cyclic Voltammetry : Principle, instrumentation, reversible and irreversible cyclic voltammograms. Applications. Cyclic voltammetric study of insecticide parathion.

II: Thermal Analysis: Thermal techniques-Introduction, types of thermo analytical methods. Thermogravimetry principle and applications of thermogravimetry.

Differential thermalanalysis- principle and applications of DTA.

Differential scanning calorimetry. DSC: Principle and applications of DSC.

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

^{1}H,^{19}F,^{31}P and solid state NMR spectroscopy: First order and non first order spectra e.g.,AX,AX_2,AX_3, A_2X_3,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,[η^5-C_5H_5M],[η^5-$(C_5H_5)_2Ti\eta^1$-$(C_5H_5)_2$] and [$\eta^4C_8H_8Ru(CO)_3$].

^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F,^{1}H and ^{31}P: 1,2 dichloro-1,1 difluoro ethane, BrF_5, SF_4, PF_5, ClF_3, IF_5, HF_2^-.

^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P , ^{19}F, ^{1}H and ^{13}C: ATP, Ph_3PSe, P_4S_3, $P(OCH_3)_3$, H_3PO_4, H_3PO_3, H_3PO_2, HPF_2, PF_6^-, PH_3,[Rh $(PPh_3)Cl_3$] Rh I=1/2

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

ASP 07: Mass spectrometry **15hrs**

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 sprectroscopy **15hrs**

Photoelectron Spectroscopy: Principle and Instrumentation, Types of Photoelectron spectroscopy – UPS & XPS Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, , CO, HF, NH_3 and H_2O - Vibrational

Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M^+) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Electron Spin Resonance Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy, quadrupolar interactions. Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bissalcylaldimine, Bis-acetylacetanatovanadyl(II) and hexachloroiridium(IV) complexes.

References:

1. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
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
6. Biological Mass Spectrometry by A.L. Burlingame
7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
8. Spectrscopic identification of organic compounds by R.M.Silverstein. G.C.Bassler and T.E.Morrill
9. NMR-A multinuclear introduction by William Kemp
10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
11. Principles of Polarography, Heyrovsky.
12. Principles of Polarography, Kapoor.
13. Modern Electroanalytical methods, edited by C.Charlot, Elsevier Company.
14. Principles of Instyrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
15. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders college Publishing.
16. Prinicples of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
17. International series of Monographs, Vol. 53: Photoelectron Spectroscopy, Edited by D. Beckerand D. Betteridge 1972.
18. Sructural methods in inorganic chemistry, E.A.V. Ebsworth.

Paper CH 251P : Inorganic chemistry-2 practicals: 6 hrs/ week

I. One component gravimetric estimations. (Use of sintered glass crucible)

(i) Estimation of Zn^{2+}.
(ii). Estimation of Ba^{2+}.

II. 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 Ag^{+} and Ca^{2+} in a mixture and estimation of Ag^{+} (gravimetric) and Ca^{2+} (volumetric).
(iii). Separation of Al^{3+} and Fe^{3+} in a mixture and estimation of Al^{3+} (gravimetric) and Fe^{3+}(volumetric).

III. Analysis of three component mixtures:

(i). Separation of (Fe^{2+} and Ni^{2+}) from Zinc (Zn^{2+}) in the given mixture and estimation ofZinc (Gravimetric).
(ii). Separation of (Ni^{2+} and Cu^{2+}) from Mg^{2+} in the given mixture and estimation of Mg^{2+}(Gravimetric).

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+}andZn^{2+}.

Suggested Books :

1. Text book of Quantitative Inorganic Analysis by A.I.Vogel, 3rd edition, ELBS 1969.
2. Vogel's text book of Quantitative Inorganic analysis. Jeffery etal, 4th edition, ELBS1988.
3. Vogel's text book of Quantitative Inorganic Analysis. 6 th edition, Pearson educationLtd. 2002.
4. Practical Inorganic chemistry By G.Marr and R.W.Rockett 1972.
5. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work. By Mounir A.Malati, 1999.
6. Advanced experimental Inorganic chemistry by. Ayodhya Singh.
7. Practical Inorganic Chemistry by G.Pass & H. Sutchiffe, 2nd edn John Wiley &Sons.

Paper CH 252P : Organic Chemistry Lab: 6 hrs / week

Systematic qualitative analysis of organic compounds

Physical data: BP / MP, Ignition test, Lassaigne's test – detection of Nitrogen, Sulphur and halogens. Solubility test for classification. Functional groups tests, Preparation of crystalline derivatives and determination of their melting points and correlation with reported data.

Study of a minimum **10** compounds covering different functional groups and solubility pattern. Glucose, benzoic acid, 2-chloro benzoic acid, anisic acid, p-nitrobenzoic acid, p-cresol, chlorophenol, β-naphthol, aniline, o/m/p-chloroanilines, N-methylaniline/N-ethylaniline, N,N-dimethyl aniline, benzamide, acetanilide, benzaldehyde, anisaldehyde, acetophenone, benzophenone, ethylbenzoate, methylbenzoate, nitrobenzene, chlorobenzene, bromobenzene, naphthalene, biphenyl and anthracene.

Introduction to structural elucidation of organic compounds by (IR, UV, ^{1}H NMR and Mass) Spectral data.

References

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.
3. Spectral identification of organic compounds Bassler, Silverstein 5th Edition.

Paper CH 253P : Physical Chemistry Lab: 6 hrs /week

Distribution:

1) Distribution of I_2 between hexanes / cyclo hexanes / CCl_4 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 [$S_2O_8^{2-}$] by initial rate method

Condutometry:

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 Fe^{+2} vs $Cr_2O_7^{-2}$ (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 $CuSO_4$ and $KMnO_4$ solutions

pH metry:

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
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical chemistr: J.B.Yadav
6. Vogel Text book of Quantitative Analysis, 6th edition, Pearson education Ltd. 2002.