# Telangana University

## M.Sc Chemistry - I Year Syllabus

# Osmania University
## M.Sc Chemistry
## Scheme of Instruction and Examination (Revised 2008) for the Batch admitted in academic year 2008-09
(Approved by the Board of Studies in Chemistry PG on 7.3.2008)

**Semester – I**

| Sub-Code | Subject | Instruction Hrs /Week | Internal Assessment Marks | Max Marks Semester Exams | Duration of semester Exam (Hrs) |
|---|---|---|---|---|---|
| | **THEORY** | | | | |
| CH-101 | Inorganic Chemistry | 4 Hrs | 20 | 80 | 3 hrs |
| CH-102 | Organic Chemistry | 4 Hrs | 20 | 80 | 3 hrs |
| CH-103 | Physical Chemistry | 4 Hrs | 20 | 80 | 3 hrs |
| CH-104 | Mathematics, Biology & Spectroscopy | 4 Hrs | 20 | 80 | 3 hrs |
| | **PRACTICAL** | | | | |
| CH-151 | Inorganic Chemistry Lab – I | 6 Hrs/week | - | - | - |
| CH-152 | Organic Chemistry Lab – I | 6 Hrs/week | - | - | - |
| CH-153 | Physical Chemistry Lab – I | 6 Hrs/week | - | - | - |
| CH-199 | SEMINAR | 2 Hrs/week | - | - | - |
| | Total | 34 + 2 | 80 | 320 | |

**Note:**

1. The candidate who studied B.Sc with Mathematics or Botany / Zoology as one of the three equal optionals must be allotted Roll number / Hall ticket number of different range.
   i. Those who have studied Mathematics at B.Sc level must study Biology in paper CH104 and be allotted Roll Number / Hall ticket number from MNO-YC-42-001 to MNO-YC-42-050.
   ii. Those who have studied Botany / Zology at B.Sc level must study Mathematics in paper CH104 and be allotted Roll Number / Hall ticket number from MNO-YC-42-051 to MNO-YC-42-100.

2. The Controller of Examination is requested to print separate D-Form for Hall-Ticket number range MNO-YC-42-001 to MNO-YC-42-050 (for Biology & Spectroscopy) and MNO-YC-051 to MNO-YC-42-100 (for Mathematics & Spectroscopy) so that the answer booklets are packed separately in the examination centre which would facilitate smooth valuation.

3. Practical examination for papers CH 151 and CH 152 and CH153 is conducted at the end of semester II along with the practical work done in semester II.

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**Semester – II**

| Sub-Code | Subject | Instruction Hrs /Week | Internal Assessment Marks | Max Marks Semester Exams | Duration of semester Exam (Hrs) |
|---|---|---|---|---|---|
| | **THEORY** | | | | |
| CH-201 | Inorganic Chemistry | 4 Hrs | 20 | 80 | 3 hrs |
| CH-202 | Organic Chemistry | 4 Hrs | 20 | 80 | 3 hrs |
| CH-203 | Physical Chemistry | 4 Hrs | 20 | 80 | 3 hrs |
| CH-204 | (A) Computers<br>(B) Spectroscopy | 4 Hrs | 20 | 80 | 3 hrs |
| | **PRACTICAL** | | | | |
| CH-251 | Inorganic Chemistry Lab | 6 Hrs/week | - | 100 | 6 hrs |
| CH-252 | Organic Chemistry Lab | 6 Hrs/week | - | 100 | 6 hrs |
| CH-253 | Physical Chemistry Lab | 6 Hrs/week | - | 100 | 6 hrs |
| CH-299 | SEMINAR | 2 Hrs/week | - | - | |
| | Total | 34 + 2 | 80 | 620 | |

**Note:**

- Practical examination in CH 151 and CH 251 is for 100 marks held at the end of semester II
- Practical examination in CH 152 and CH 252 is for 100 marks held at the end of semester II
- Practical examination in CH 153 and CH 253 is for 100 marks held at the end of semester II

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# M.Sc CHEMISTRY REVISED SYLLABUS
## (To be implemented for the batch admitted in 2008-2009)
## (Approved by the P.G. Board of Studies on 7th March 2008)

## SEMESTER –I

Semester -I and Semester-II syllabus is common for all specializations i.e., Inorganic-Analytical, Organic, Physical, Analytical and Physical- Organic

**Paper 1 CH ... (INORGANIC CHEMISTRY)**
Unit IC 01: Bonding in metal complexes-I
Unit IC 02:Reaction mechanism of transition metal complexes
Unit IC 03:Coordination equilibria
Unit IC 04:Ligational aspects of diatomic molecules

Teaching hours/week-4 Marks-80

**IC – 01: Bonding in metal complexes – I:**
Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular Octahedral, tetragonally distorted octahedral, Jahn-Tellar theorem-, tetrahedral, square planar, trigonal planar, 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-02: 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.
Substitution reactions with out 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 $\pi$ - 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.

**IC-03: Coordination Equilibria:**
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)

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– 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:**

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; Classification in to Low Nuclearity and High Nuclearity carbonyl clusters; 18 Valence electron rule and its application to Low Nuclearity carbonyl clusters; Structures of $Ni(CO)_4$ , $Cr(CO)_6$ , $Mn_2(CO)_{10}$ , $Fe_2(CO)_9$ and $Co_2(CO)_8$ ; Structures of Low nuclearity

$M_3(CO)_{12}$ ( M=Fe,Ru,Os) and $M_4(CO)_{12}$ (M=Co,Rh,Ir).

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.

**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. Preparation of complexes:

(i). Hexaammine nickel (II) chloride.
(ii). Tris (acetylacetanato) manganese.
(iii). Tris (ethylenediamine) nickel (II) thiosulphate.
(iv). Mercury tetrathiocyanato cobaltate (II).

V. Preparation of complexes and calculation of % purity:

(i). Tetrammine copper (II) sulphate and estimation of $NH_3$ and calculation of % purity.
(ii). Pentaammine (chloro) cobalt (III) chloride and estimation of $Cl^-$ and calculation of % purity.
(iii). Sodium trioxalato ferrate (III) and estimation of $C_2O_4^{2-}$ and $Fe^{2+}$ and calculation of % purity.

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**Paper 2 CH 102 (ORGANIC CHEMISTRY)**

OC 01:Stereochemistry-I
OC 02:Reaction mechanism-I
OC 03:Carbohydrates and Proteins
OC 04:Heterocyclic compounds

Teaching hours/week-4 Marks-80

**OC 01:Stereochemistry-I**

**Symmetry**: Symmetry elements in methane, staggered ethane, ethylene, benzene, chair cyclohexane, allene, tartarc acids. Point groups: Achiral and chiral point groups and their symmetry elements. Desymmetrization.

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

**Relative and absolute configuration**: Determination of absolute configuration Anamolous X- ray scattering method and chemical correlation methods.

**Properties of enantiomers and diastereoisomers**;Discrimination of enantiomers based on diastereomeric interactions, chiroptical methods, chiral NMR solvents, chiral stationary phases and enzymes.

**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 chemical methods of configuration determination of E,Z isomers. Determination of configuration in aldoximes and ketoximes.

**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 $OsO_4$ and $KMnO_4$

**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, crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

**OC 03:Carbohydrates and Proteins**

**Carbohydrates:** Determination of the relative and absolute configuration in D (+) glucose and D (-) fructose.Proof for the chair conformation of D (+) glucose. Occurence, importance and synthesis of monosaccharides containing functional groups such as amino,halo and sulphur.Structure elucidation and synthesis of sucrose.Conformational structures of D(+) ribose,2- deoxy D-ribose, sucrose, lactose maltose and cellobiose.Structural features of starch, cellulose and chitin.

**Proteins:** Acid and enzymatic hydrolysis of proteins.Determination of the amino acid sequence in polypeptides by end group analysis.Chemical synthesis of di and tripeptides. Merrifield's solid phase synthesis.

**QC 4:Heterocyclic compounds**

**Heterocyclic compounds**

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, Interscience Publishers, New York, 1967.
8.Advanced Organic Chemistry by Jerry March
9.Mechanism and Structure in Organic Chemistry S. Mukerjee

**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-nitroaniline, hippuric acid, azlactone,anthracene-maleic anhydride adduct, Phthalimide, 2,4-dihydroxyacetophenone

**Demonstration experiments:**

1.Synthesis of organic compounds by use of microwave oven.(any two examples)
2.Quantitative estimations by colorimetry.( one example)
3.Thin layer chromatography to moniter chemical reactions.( all 15 compounds synthesized above)
4.Steam distillation technique in the separation of o- and p- nitro phenols.

**References.**

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

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**Paper CH 103 ( PHYSICAL CHEMISTRY)**

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

Teaching hours/week-4

Marks-80

**PC-01: Thermodynamics-I**

Brief review of concepts of I and II laws of thermodynamics. Concept of entropy-entropy as a state function. Entropy changes in various processes. Entropy changes in an ideal gas. Entropy changes on mixing of ideal gases. 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 energies(A and G) A and G as criteria for equilibrium and spontaneity. Physical significance of A and G. Driving forces for chemical reactions-relative signs of $\Delta H$ and $\Delta S$.

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 equilibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.

**PC-02:Electrochemistry-I**

**Elecrochemical cells.** Derivation of Nernst equation- problems. Chemical cells and concentration cells with and without transference. Liquid junction potential and its determination. Potentiometric titrations, determination of pH and solubility product from emf measurements.

**Electrode polarization**, decomposition potential, over voltage and its applications. Concentration over potential

**Principles of polarography**-DME, Ilkovic equation(derivation not required), polarogram-description and equation for a polaogram. Diffusion current, half wave potential and its significance, Fick's I law of diffusion. Nernst hypothesis- thickness of diffusion layer. Applications.

Principle and applications of amperometric titrations and determination of $SO_4^{2-}$, metal ions

viz.,$Mg^{2+}$ ,$Cu^{2+}$ and $Zn^{2+}$ . Principles of cyclic voltametry. Cyclic voltametric study of insecticide parathion.

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

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 $\nabla$ and $\nabla^2$ . 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.

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

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( $\sigma$ and $\sigma^*$) and reaction constant ( $\rho$ and $\rho^*$ )with examples. Deviations from Hammett correlations reasons-Change of mechanism, resonsnce 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 intrinsic barrier and 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. Principles of Polarography, Herovsky
11. Principles of polarography, Kapoor
12. The Physical Basis of Organic Chemistry by Howard Maskill, Oxford University Press (New York)

**Paper 153 Physical Chemistry Lab course 6 hours/ 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 $CCl_4$ 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

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**Paper 4 CH 104 (MATHEMATICS/BIOLOGY and SPECTROSCOPY)**
M/B 01:Maths/Biology
SP 02: NMR spectroscopy-I ($^1$H NMR)
SP 03:Rotational and Vibrational spectroscopy
SP 04:Electronic spectroscopy

Teaching hours/week-4 Marks-80

**M/B-01: Mathematics (for students without mathematics in B.Sc)**

**Coordinate system**- . Graphical representation of the functions:
$y = e^x$, $y = \ln x$, $y = kx^2$, $y = \sin x$, $y = \cos x$, $y = \tan x$.

**Differential calculus:** Functions-continuity and differentiability. Rules for differentiation. Sums, products and quotients of functions. The chain rule. Differemiation of algebric, exponential,logarithemic and composite functions. Higher-order derivatives. Maxima and minima. Partial differentiation and meaning of total derivative. Exact and inexact differentials

**Integral calculus:** basic rules for integration. Methods for evaluating integrals-the substitution method, use of partial fractions, integration by parts. Definite integrals.

**Elementary differential equations**: First order differential equations-separable variables, homogeneous and linear differential equations. Linear second order differential equations-solution of the homogeneous equation.

**M/B 01 Biology (For students without biology in B.Sc):**

**Cell Biology:**Prokaryotes, Eukaryotes, Sub cellular organelles and their functions, (cell membrane,mitochondria, lysosomes,nucleus, chromosomes etc).Staining,Marker enzymes. Cell specialization: muscle and nerve.

Metabolicprocess: anabolism and catabolism,biological role of ATP,Glycolysis, glycogenolysis, glycogenesis , Kreb's cycle

Nucleic acids:Structure of bases, stretures of nucleosides and nucleotides.Structure of DNA and RNA,double helix structure of DNA.Gene,genome.Replication,Protein biosynthesis,transcription, translation, Genetic code, mutation, phenotype and genotype.

**Immune system:**Functions of immune system, primary and secondary immune responses, polyclonal and monoclonal antibodies.ELISA, Western blotting.AIDS

**SP 02: NMR spectroscopy-I ($^1$H NMR)**

**$^1$H NMR spectroscopy:** Magnetic properties of nuclei, Principles of NMR. Instrumentation. CW and FT NMR, 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,long range and virtual coupling.Coupling constants and factors affecting coupling constants.

Applications of $^1$H NMR spectroscopy: structure determination, 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 process, C-N rotation, study of aromaticity and fluxional molecules (eg.,bullvalene,$[\eta\text{-}C_5H_5M]$,$\eta\text{-}(C_5H_5)_2$ $Ti\eta\text{-}(C_5H_5)_2$ $[\text{-}C_8H_8Ru(CO)_2]$.NMR of paramagnetic compounds:$[H\ Ni(OPEt_3)_4]$,$[HRh(CN)_5]^{3-}$

acetylacetone complexes.Problems based on $^1H$ NMR spectral data,.magnetic resonance imaging(MRI).

**SP 03 :Rotational and Vibrational spectroscopy**

**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 bondlengths 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. Problems based on group frequencies. Applications of IR spectroscopy to the study of metal-ligand bonding modes involving monodentate amd bidentate ligands. IR spectra of coordinated $NO_3^-$, $SO_4^{2-}$ and $CO_3^{2-}$ ions.

**Raman Spectroscopy-** Quantum theory of Raman effect, Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

**SP 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 and its derivatives, Woodward-Fieser rules. Polynuclear aromatic hydrocarbons and diketones. Solvent and structural influences on absorption maxima, stereochemical factors. Cis-trans isomers, and cross conjugation. Application of electronic spectra of metal complexes-"$3d^1$ and $3d^9$ hexa aquo metal complexes. Quantitative applications of electronic spectroscopy, Beer's law application to mixture analysis and dissociation constant of a weak acid, Charge transfer spectra

**References:**

1. Mathematical preparation for Physical Chemistry, F. Daniels, McGraw Hill
2. Mathematics for Chemistry, Doggett and Sutcliffe, Longman
3. Mathematics for Chemists, D.M. Hirst, MacMillan
4. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
5. Introduction to Molecular Spectroscopy, G.M. Barrow
6. Absorption Spectroscopy of Organic Compounds, J.R. Dyer
7. Biochemistry: Hames and Hooper
8. Genetics : Winter, Hickey and Fletcher
9. Biotechnology: Balasubramanian.
10. Molecular biology : Turner, Mc Lennen, Bates and White.

## SEMESTER -II

Semester -I and Semester-II syllabus is common for all specializations i.e., Inorganic-Analytical, Organic, Physical, Analytical and Physical- Organic

**Paper CH 201 INORGANIC CHEMISTRY**

IC 05:Symmetry of molecules
IC 06: Bonding in metal complexes-II
IC 07:Metal clusters
IC 08:Biocoordination chemistry

Teaching hours/week-4 Marks-80

**IC-05: Symmetry of Molecules:**

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 Dipole moment – Symmetry criteria for Optical activity..

**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 – electron repulsion Parameters ( Racah parameters) – Spin-Orbital coupling parameters. Effect of weak cubic crystal fields on S,P,D and F terms- Orgel Diagrams.

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- Relative stability of Bridging and Non- bridging structures . 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 $[Os_6(CO)_{18}]^{2-}$ , $[Rh_6(CO)_{15}]$, $[Os_7(CO)_{21}]$ , $[Rh_7(CO)_{16}]^{3-}$, $[Os_8(CO)_{22}]^{2-}$ , $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_6(CO)_{12}]^{2-}$. Stereo chemical non- rigidity (Fluxionality) in $Cp_3Rh_3(CO)_3$, $Rh_4(CO)_{12}$ clusters. Interconversion of Cis-Trans isomers of $Cp_2Fe_2(CO)_4$.

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 $[Re_2Cl_8]^{2-}$ 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.

**IC-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 and Myoglobin: Geometric, electronic and magnetic aspects of Dioxygen binding, Oxygen adsorption isotherms and cooperativity in Hemoglobin and its physiological significance. Role of globin chain. Hemerythrin and Hemocyanin: Structure of deoxy forms, oxygen binding, Geometric, electronic and magnetic aspects. Comparison of Hemerythrin and Hemocyanin with hemoglobin.

Photosynthesis: Structural aspects of Chlorophyll. Photo system I and Photo system 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.

**Semester II: Inorganic chemistry practicals**

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

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

(ii). Estimation of $Ba^{2+}$ (as $BaSO_4$).

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).

III. Analysis of three component mixtures:

(i). Separation of ($Fe^{2-}$ and $Cu^{2+}$) from Zinc ($Zn^{2+}$) in the given mixture and estimation of Zinc (Gravi).

(ii). Separation of ($Ni^{2+}$ and $Cu^{2+}$) from $Mg^{2+}$ in the given mixture and estimation of $Mg^{2+}$ (Gravi).

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 $Zn^{2+}$.

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**Textbooks and References Recommended for Theory (For both semesters).**

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. Inorganic Reaction Mechanisms. M.L.Tobe and John Burgess, Addison Wesley Longman (1999).

5. Metal ions in Reaction Mechanisms. K.Veera Reddy. Golgotia Publications (P) Ltd (2004).

6. Mechanisms of Reactions in Transition Metal Sites. Richard A Henderson, Oxford Science Publications, London (1993).

7. Inorganic Reaction Mechanisms, F.Basolo and R.G.Pearson, New York (1967).

8. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6 Th Edition, Wiley Interscience, N.Y (1999

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9. Inorganic Chemistry. J.E.Huheey , K A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
10. Inorganic Biochemistry Edited by G.L.Eichorn, Volume I Elsevier ( 1982).
11. Homogeneous Catalysis by Metal complexes Vol I. M M Taqui Khan and A E Martell, Academic Press NY (1974).
12. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
13. Inorganic Chemistry. Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions. London (1977).
14. Bioinorganic Chemistry. I.Bertini, H.B.Gray, S.J.Lippard and S.J.Valentine, Viva Low-Priced Student Edition. New Delhi (1998).
15. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life. W.Kain and B.Schwederski, John Wiley and Sons, NY (1999).
16. Bioorganic Chemistry – Dugas.

**Books Recommended for practicals**: (For both semesters).

I. (i). Text book of Quantitative Inorganic Analysis by A.I.Vogel, 3rd edition, ELBS 1969.

(ii). Vogel's text book of Quantitative Inorganic analysis. Jeffery etal, 4th edition, ELBS 1988.

(iii). Vogel's text book of Quantitative Inorganic Analysis. 6 th edition. Pearson education ltd 2002.

II. Practical Inorganic chemistry By G.Marr and R.W.Rockett 1972.

III. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work. By Mounir A.Malati, 1999.

IV. Advanced experimental Inorganic chemistry by. Ayodhya Singh.

**Paper CH 202 ORGANIC CHEMISTRY**

OC 05: Conformational analysis (acyclic systems)
OC 06: Reaction mechanism-II
OC 07 : Reactive intermediates and Molecular rearrangements.
OC 08: Natural products (Terpenoids and Alkaloids).

**OC 05: Conformational analysis (acyclic systems)**

Introduction to conformational isomerism and the concept of dynamic stereochemistry.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).Conformational diastereoisomers and conformational enantiomers -. 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 stereo electronic factors-examples.Conformation and reactivity: The Winstein-Holness equation and the Curtin – Hammett principle.

**OC 06: Reaction mechanism-II**

**Nucleophilic Aromatic substitution:**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.

**Neighboring group participation** : Criteria for determining the participation of neighboring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. Neighboring group participation involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl, Cycloalkyl groups, $\sigma$ and $\pi$- bonds. Introduction to nonclassical carbonium ions.

**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 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: Wagner- Meerwein, Pinacol-Pinacolone, Allylic and Wolf rearrangement. 2) electron deficient Nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements 3) electron deficient Oxygen: Baeyer-Villiger oxidation. 4) Base catalysed rearrangements: Benzilic acid , Favourski , Transannular , Sommlett-Hauser and Smiles rearrangement

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**OC 08: Natural products (Terpenoids and Alkaloids).**

**Natural products –1**

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.Advanced Organic Chemistry by Jerry March
7.Mechanism and Structure in Organic Chemistry S. Mukerjee
8.Organic chemistry Vol.I and II by I.L.Finar
9.Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D..Ollis

**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-Ethyl aniline, N,N-Dimethyl aniline, Benzamide, Benzaldehyde, Anisaldehyde,

Acetophenone,benzophenone,Ethylbenzoate,methylbenzoate,Nitrobenzene, chlorobenzene, bromobenzene , naphthalene, biphenyl, anthracene.

**Identification of unknown organic compounds from their IR,UV,$^1$H 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
2. Text book of practical organic chemistry, Mann and Saunders.
3.Spectral identification of organic compounds Bassler. Silverstein 5th Edition

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**Paper CH 203 PHYSICAL CHEMISTRY**

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

**PC-05:Thermodynamics-II**

Solutions. Partial molar poperties-significance. Relation between solution volume and partial molar volumes.Determination of partialmolar volumes-slope and intercept methods. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance

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 nonideal solutions. Excess functions and their determination. 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.

**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. Actinometry-ferrioxalate and uranyl oxalate actinometers-problems.

Derivation of fluorescence and phosphorescence quantum yields. E-type delayed fluorescence- evaluation of triplet energy splitting($\Delta E_{ST}$). 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**

*Particle in a box*- one dimensional and three dimensional. Plots of $\psi$ and $\psi^2$-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.

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 pots 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. Particle 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 variationan 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 wave function and the energy of $H_2$ molecule MO by LCAO method and Valence bond method (detailed calculations not required). Comparison of MO and VB models.

**PC-08: Solid state chemistry**

**Solid state reactions**.-classification . kinetics of solid state reactions. Crystal defects. Perfect and imperfect crystals. Classification of imperfections. Point defects. Schotky defects, Frenkel defects. Line defects and plane defects.

**Electronic properties of metals, insulators and semi conductors** electronic structure of solids, Band theory, band structure of metals, insulators and semiconductors. Electrons and holes 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 pyrovskites. High $T_c$ superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_{7-x}$. Preparation and characterization of 1-2-3 materials. Origin of high $T_c$ superconductivity.

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. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan
8. Introduction to Electrochemistry, S. Glasstone
9. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
10. Solid state Chemistry, D.K. Chakrabarthy, New Age International
11. Solid state Chemistry and its aplications, A.R. West, Plenum.
12. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
13. Molecular Photochemistry, N.J. Turro, Benjamin
14. Photochemistry, R.P.Kundall and A. Gilbert, Thonson Nelson

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15. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
16. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
17. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.

**Paper CH 253 (Physical Chemistry Lab)**

**Distribution:**

1) Distribution of $I_2$ between $CCl_4$ 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

**Solutions:**

1)Determination of molecular weight of a non volatile substance by cryoscopic method
2)Determination of degree of dissociation by cryoscopic method
3)Study of surface tension-concentration relationship for solutions (Gibbs equation)

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**Paper CH 204 COMPUTERS and SPECTROSCOPY**

CO-05: Computers for Chemists.
SP-06: NMR II
SP-07: Mass Spectroscopy-I
SP-08: Mass Spectroscopy-II

**CO-05: Computers for Chemists (15 hrs)**

Introduction to computers (Input and Output devices, central processing unit) software and computer languages. Algorithms and flow charts.

**C language** instructions. Constants, variables and key words.

Operators in C – arithmetic, relational, logical and address operators. Library functions. Detailed information about -input and output functions- printf( ), scanf ( ),gets ( ),puts ( ).

Control Statements -If and If-else statements. Loops- While loop and For loop.

Functions – Defining a function. Accessing a function.

Arrays – Defining an array. Processing an array. Passing arrays to functions. Two dimensional arrays.

Steps in testing a source program in C.

C language programs for:

1. Roots of a quadratic equation
2. First-order rate constant from kinetic data
3. Summation of a series
4. Least-square fitting of XY data to a straight line
5. Calculation of activation energy using Arrhenius equation by least-square fitting
6. Calculation of energy as a function of inter nuclear separation for $H_2^+$ ion
7. Dissociation constant of acetic acid from conductance data
8. $\Psi$ and $\Psi^2$ values at different x for a particle in a one-dimensional box

**SP 06: ; NMR spectroscopy-II ($^1H$,$^{19}F$ and $^{31}P$ NMR)**

**$^1H$,$^{19}F$,$^{31}P$ 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

Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid.

Simplification of complex spectra: increased field strength, deuterium exchange,Lanthanide shift reagents and double resonance techniques. Nuclear Overhauser enhancement (NOE)..

$^{19}F$ NMR spectroscopy: $^{19}F$ chemical shifts, coupling of $^{19}F$ with $^{19}F$,$^1H$,$^{13}C$ and $^{31}P$.Applications of $^{19}F$ NMR.

$^{31}P$ NMR spectroscopy: $^{31}P$ chemical shifts, coupling of $^{31}P$ with $^{31}P$ ,$^{19}F$,$^1H$ and $^{13}C$.Applications of $^{31}P$ NMR

Introduction to solid state NMR:

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

**SP 07: Mass spectrometry-I**

Origin of mass spectrum, Principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species. Nitrogen rule, Isotopic peaks, determination of molecular formula, metastable ion peaks. High

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resolution mass spectrometry. Principles of ion production techniques such as EI, CI, FI and FD methods and mass analysers such as time of flight, ion trap and quadrupole analyzer. Fast Atom Bombardment (FAB), Secondary Ion Mass (SIM) spectrometry and Californium plasma desorption techniques. Principle of Electron Spray Ionization(ESI) mass spectrometry, Matrix Assisted Laser Desorption Ionization (MALDI) mass spectrometry, GC-MS and LC-MS.

**SP 08:Mass spectrometry-II**

Common mass fragmentation pattern of organic compounds.Cleavage of one, two and more bonds. Dehydration, dehydrohalogenation, decarboxylation (eliminations).Fragmentation of alkanes, alkenes,(allylic cleavage),cycloalkanes,cycloalkenes (retro Diels-Alder fragmentation) cycloalkanols, cycloalkanones and cycloalkyl amines, alkyl substituted aromatic compounds (benzylic cleavage), phenols,aldehydes, ketones,carboxylic acids, esters, amides,amines, alcohols,McLafferty rearrangement,ortho effect.Interpretation of the fragmentation pattern of simple organic compounds.Fragmentation pattern of metal carbonyls and mass spectral fragmentation of ReBr, $ReBr_2$ and $ReBr(CO)_5$

**References:**

1. Fundamentals of Computers, Rajaraman
2. Programming with C, Schaums outlin
3. Programming in C, Rajaraman
4. Let Us C , Yashavanth Kanitker
5. Computers in Chemistry, K.V. Raman
6. Programming in C, Balaguruswamy
7.Organic spectroscopy by William Kemp
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