Scheme and Syllabus
of
M.Sc. Chemistry

I and II Semesters

Effective from Academic Year 2016-17 onwards

Devi Ahilya Vishwavidyalaya,
Indore (M.P.), 452001

DEVI AHILYA VISHWAVIDYALAYA, INDORE

Scheme of Marks

M. Sc. Chemistry

(w.e.f. 2016 and onwards)

SEMESTER – I

Paper	Compulsory/Optional	Paper Title	Code (MCH)	Max. Marks
I	Compulsory	INORGANIC CHEMISTRY	401	85+ 15(CCE) = 100
II	Compulsory	ORGANIC CHEMISTRY	402	85+ 15(CCE) = 100
III	Compulsory	PHYSICAL CHEMISTRY	403	85+ 15(CCE) = 100
IV	Compulsory	GROUP THEORY & SPECTROSCOPY I	404	85+ 15(CCE) = 100
V	For Students Without Mathematics in B.Sc.	MATHEMATICS FOR CHEMISTS	405(a)	85+ 15(CCE) = 100
	For Students Without Biology in B.Sc.	BIOLOGY FOR CHEMISTS	405(b)	85+ 15(CCE) = 100
		PRACTICAL - 1. Inorganic 2. Organic 3. Physical		33 33 34 =100
		Total		600

M. Sc. Chemistry

SEMESTER – II

Paper	Compulsory/Optional	Paper Title	Code (MCH)	Max. Marks
I	Compulsory	INORGANIC CHEMISTRY	406	85+ 15(CCE) = 100
II	Compulsory	ORGANIC CHEMISTRY	407	85+ 15(CCE) = 100
III	Compulsory	PHYSICAL CHEMISTRY	408	85+ 15(CCE) = 100
IV	Compulsory	SPECTROSCOPY II & DIFFRACTION METHODS	409	85+ 15(CCE) = 100
V	Compulsory	COMPUTER FOR CHEMISTS	410	85+ 15(CCE) = 100
		PRACTICAL - 1. Inorganic 2. Organic 3. Physical		33 33 34 =100
		Total		600

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – I)

Paper No. : I (Code-MCH-401)
Compulsory / Optional : Compulsory
Max. Marks : 100

Paper – I : Inorganic Chemistry

Unit – I	**Stereochemistry and Bonding in Main Group Compounds :** VSEPR, Walsh diagram (triatomic and penta-atomic molecules), dπ-pπ bond, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.
Unit – II	**Metal-Ligand Equilibrium in Solution** Stepwise and overall formation constants and their interaction, trends in stepwise constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by potentiometry and spectrophotometry.
Unit – III	**Reaction Mechanism of Transition Metal Complexes** Energy profile of a reaction, reactivity of metal complex, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anion reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.
Unit – IV	**Metal-Ligand bonding** Limitation of crystal field theory, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes, π-bonding and molecular orbital theory.
Unit –V	**HSAB Theory** Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; donor and acceptor numbers, E and C equation; applications of HSAB concept.

Books Suggested :

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of the Elements. N.N. Greenwood and A. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetiochemistry, R.1. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc-Cleverty,Pergamon.

2-9-2016 2-9-16 2-9-16 2/9/2016 2.9.16 5.9.2016 2/9/16

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – I)

Paper No. : **II (Code- MCH-402)**
Compulsory / Optional : **Compulsory**
Max. Marks : **100**

Paper – II : Organic Chemistry

Unit – I	**Nature of Bonding in Organic Molecules** Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, energy level of π-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compound, catenanes and rotaxanes.
Unit – II	**Stereochemistry** Strain due to unavoidable crowding, Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spirane) chirallity due to helical shape. Stereochemistry ofthe compounds containing nitrogen, sulphur and phosphorus.
Unit – III	**Conformational analysis and linear free energy relationship** Conformational analysis of cycloalkanes, decalines, effect of conformation on reactivity, conformation of sugars. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. The Hammett equation and linear free energy relationship, substituents and reaction constants, Taft equation.
Unit – IV	**Reaction Mechanism : Structure and Reactivity** Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtir-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopes effects.
Unit –V	**Aliphatic Nucleophilic Substitution** The SN^2, SN^1 mixed SN^1 and SN^2 and SET mechanism. The neighboring group mechanism, neighboring group participation by p and s bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN^1 mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

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Books Suggested :

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Comell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – I)

Paper No. : **III (Code- MCH-403)**
Compulsory /Optional : **Compulsory**
Max. Marks : **100**

Paper – III : Physical Chemistry

Unit – I	**Introduction to Exact Quantum Mechanical Results** Schrödinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrödinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom and helium atom.
Unit – II	**Approximate Methods** The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom. **Molecular Orbital Theory** Huckel theory of conjugated systems bond and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene etc. Introduction to extended Huckel theory.
Unit – III	**Angular Momentum** Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum operator using ladder operators addition of angular momenta, spin, anti-symmetry and Pauli exclusion principle.
Unit – IV	**Classical Thermodynamics** Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems : Excess function s for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.
Unit –V	**Statistical Thermodynamics** Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition. Application of partition functions. Fermi-Dirac Statistics, distribution law and applications to metal. Bose-Einstein statistics distribution Law and application to helium.

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1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R. Mc Ween y, ELBS.
5. Chemical Kinetics. K. J. Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
8. Modern Electrochemistry Vol. 1 and Vol. II J.O.M. Bockris and A.K.N. Reddy, Planum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
10. Introduction to Quantum Chemistry-R.K. Prasad, New Age Publication.

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – I)

Paper No. : **IV (Code-MCH-404)**
Compulsory / Optional : **Compulsory**
Max. Marks : **100**

Paper – IV : Group Theory & Spectroscopy I

Unit – I	**Symmetry and Group theory in Chemistry** Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schonfilies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} group to be worked out explicity). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Derivation of character table for C_{2v} and C_{3v} point group Symmetry aspects of molecular vibrations of H_2O molecule.
Unit – II	**Microwave Spectroscopy** Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.
Unit – III	**Infrared Spectroscopy** Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. P.Q.R. branches, Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal ligand vibrations, normal co-ordinate analysis.
Unit – IV	**Raman Spectroscopy** Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, coherent anti stokes Raman spectroscopy (CARS).
Unit –V	**Electronic Spectroscopy** **Molecular Spectroscopy** Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radio-active and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra. **Photoelectron Spectroscopy** Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy-basic idea.

oks suggested:

1. Modern Spectroscopy, J.M. Hollas, John Viley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH- Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper & Row.

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – I)

Paper No. : **V [Code-405(a)]**
Compulsory / Optional : **Compulsory**
Max. Marks : **100**

Paper – V : (a) Mathematics For Chemists

(For students without Mathematics in B.Sc.)

Unit – I	**Vectors** Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus. **Matrix Algebra** Addition and multiplication; inverse, adjoint and transpose of matrices.
Unit – II	**Differential Calculus** Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.).
Unit – III	**Integral Calculus** Basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).
Unit – IV	**Elementary Differential equations** First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.
Unit –V	**Permutation and Probability** Permutations and combinations, probability and probability theorems average, variance root means square deviation examples from the kinetic theory of gases etc., fitting (including least squares fit etc with a general polynomial fit).

Books suggested

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematics for chemistry, Doggett and Suiclific, Logman.
3. Mathematical for Physical Chemistry : F. Daniels, Mc. Graw Hill.
4. Chemical Mathematics D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.

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M.Sc. CHEMISTRY (SEMESTER – I)

Paper No. : **V [Code-405(b)]**
Compulsory / Optional : Compulsory
Max. Marks : 100

Paper – V : (b) Biology For Chemists

(For students without Biology in B.Sc.)

Unit – I	**Cell Structure and Functions** Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview and their functions, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism. ATP - the biological energy currency. Origin of life-unique properties of carbon chemical evolution and rise of living systems. Introduction to bio-molecules, building blocks of bio-macromolecules.
Unit – II	**Carbohydrates** Conformation of monosaccharides, structure and functions of important derivatives of mono-saccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides. Carbohydrates of glycoporteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.
Unit – III	**Lipid** Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Liproproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism-β-oxidation of fatty acids.
Unit – IV	**Amino-acids, Peptides and Proteins** Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins. Force responsible for holding of secondary structures. α-helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination : chemical / enzymatic / mass spectral, racemization /detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).
Unit –V	**Nucleic Acids** Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of

	nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

Books suggested :

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawan, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry E.E. Conn and P.K. Stumpf, John Wiley.

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M. Sc. CHEMISTRY PRACTICALS (SEMESTER – I)

Practical examination shall be conducted separately for each branch : (Duration : 6-8 hrs in each branch).

Inorganic Chemistry

Qualitative & Quantitative Analysis		12
Chromatography		06
Preparation		06
Record		04
Viva Voce		05
	Total :	33

Qualitative Analysis :

(a) Analysis of Less common metal ions : W, Mo, Se, Ti, Zr, Ce, V, etc. (Two metal ion in cationic / anionic forms).

(b) Analysis of Insoluble residue : Oxides, sulphates & halides.

Quantitative Analysis : Separation & estimation of two metal ions viz., Cu – Zn, Fe – Mg, Ni – Zn, etc. involving volumetric & gravimetric methods.

Chromatography: Separation, identification & determination of cations & anions by Paper Chromatography.

Preparations : Preparation of selected inorganic complexes, their analysis, test & characterization by spectral techniques (may be).

(1) $VO(acac)_2$.

(2) $Ni(acac)_2$.

(3) $[Co(NH_3)_6]Cl_3$.

(4) $NH_4[Cr(NH_3)_2(SCN)_4]$ … Reinecke's salt.

(5) Prussian Blue ; Turnbull's Blue.

(6) Oxalate complexes of Chromium (III) & Copper (II).

Organic Chemistry

Qualitative Analysis	12
Organic Synthesis	12
Record	04
Viva-Voce	05
Total :	33

Qualitative Analysis : Separation, purification & identification of compounds of ternary mixture (solid or solid + liquid) using TLC & columns chromatography, chemical tests. IR spectra to be used for functional group identification.

Organic Synthesis :
Acetylation, Nitration, Halogenation, Oxidation, Reduction, Polymerization.

Physical Chemistry

Any **one** Experiment / Exercise from **Section – A**	12
Any **one** Experiment / Exercise from **Section – B**	13
Record	04
Viva-Voce	05
Total :	34

Section – A

Error Analysis & Statistical Data Analysis
Errors, types of errors, minimization of errors distribution curves precision, accuracy & combination; statistical treatment for error analysis, student's t-test, null hypothesis, rejection criteria. F & Q – test; linear regression analysis, curve fitting. Calibration of volumetric apparatus : Burette, pipette & standard flask.

Adsorption : To study surface tension – concentration relationship for solutions (Gibb's equation).

Phase Equilibria :

(i) Determination of congruent composition & temperature of a binary system (e.g., diphenylamine – benzophenone system).

(ii) Determination of glass transition temperature of given salt (e.g., $CaCl_2$) conductometrically.

(iii) To construct the phase diagram for three component system (e.g., chloroform – acetic acid – water).

Section – B

Chemical Kinetics :

(i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactant & catalyst & (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reaction.

(ii) Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media.

(iii) Determination of the velocity constant for the oxidation of iodide ions by hydrogen peroxide. Study the kinetics as an iodine clock reaction.

(iv) Flowing clock reactions (Ref : Experiments in Physical Chemistry by Showmaker).

(v) Determination of the primary salt effect on the kinetics of ionic reaction & testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

Solution:

(i) Determination of molecular weight of non – volatile & electrolyte / electrolyte by cryoscopic method & to determine the activity coefficient of an electrolyte.

(ii) Determination of the degree of dissociation of weak electrolyte & to study the deviation from ideal behavior that occurs with a strong electrolyte.

Books Suggested

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly. Prentice Hall.
3. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall.
4. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Health.
5. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
6. Handbook of Organic Analysis-qualitative and Quantitative. H. Clark, Adward Arnold.
7. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
8. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
9. Findley's Practical Physical chemistry, B.P. Levitt, Longman.
10. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – II)

Paper No. : **I (Code-MCH-406)**
Compulsory /Optional : **Compulsory**
Max. Marks : **100**

Paper – I : Inorganic Chemistry

Unit – I	**Electronic Spectral Studies of Transition Metal Complexes :** Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), Selection rule for electronic spectroscopy. Intensity of various type electronic transitions. Calculations of 10Dq, B and β parameters, charge transfer spectra.
Unit – II	**Magnetic Properties of Transition Metal Complexes** Anomalous magnetic moments, Quenching of Orbital contribution. Orbital contribution to magnetic moment, magnetic exchange coupling and spin crossover.
Unit – III	**Metal π-Complexes** Metal carbonyl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reaction of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.
Unit – IV	**Metal-Clusters** Higher boranes, carboranes, metalloboranes and metallo-carboranes compounds with metal-metal multiple bonds.
Unit –V	**Optical Rotatory Dispersion and Circular Dichroism** Linearly and circularly polarized lights; optical rotatory power and circular birefringence, elipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; Assignment of electronic transitions; applications of ORD and CD for the determination of (i) absolute configuration of complexes and (ii) isomerism due to non-planarity of chelate rings.

Books Suggested :

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huheey, Harpes & Row.
3. Chemistry of the Elements. N.N. Greenwood and A. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetiochemistry, R.1. Carlin, Springer Verlag.
6. Comprehensive Coordiantion Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty, Pergamon.

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – II)

Paper No. : **II (Code-MCH-407)**
Compulsory /Optional : **Compulsory**
Max. Marks : **100**

Paper – II : Organic Chemistry

Unit – I	**Aromatic Electrophilic Substitution** The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gatterman-Koch reaction. **Aromatic Nucleophilic Substitution** The SNAr SN^1, benzyne and SN^1 mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richter, Sommelet-Hauser, and Smiles rearrangements.
Unit – II	**Free Radical Reactions** Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.
Unit – III	**Addition Reactions** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, sharpless asymmetric epoxidation.
Unit – IV	**Addition to Carbon-Hetero Multiple bonds** Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters. **Elimination Reactions** The E_2, E_1 and E_1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

	Pericyclic Reactions Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of periycyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n 4n+2 and allyl systems. Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotrpic reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

Books Suggested :

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Comell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
11. Stereochemisty of Organic Compounds, P.S. Kalsi, New Age International.

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – II)

Paper No. : **III (Code- MCH-408)**
Compulsory /Optional : **Compulsory**
Max. Marks : **100**

Paper – III : Physical Chemistry

Unit – I	**Chemical Dynamics** Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and homogenous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method, dynamics of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel- Marcus (RRKM) theories for unimolecular reactions).
Unit – II	**Surface Chemistry** **Adsorption** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon). **Micelles** Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solublization, micro emulsion, reverse micelles.
Unit – III	**Macromolecules** Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (Osmometry, viscometry, diffusion and light scattering methods, sedimentation), chain configuration of macromolecules, calculation of average dimension of various chain structures.
Unit – IV	**Non-Equilibrium Thermodynamics** Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction.

	Electrochemistry Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Overpotentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface. Polarography theory, Ilkovic equation; half wave potential and its significance.

Books Suggested :

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R.Mc Ween y, ELBS.
5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
6. Kinetics & Mechanism of Chemical Transformation J.Rajaraman & J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
8. Modern Electrochemistry Vol. 1 and Vol. II J.O.M. Bockris and A.K.N. Reddy, Planum.
9. Introduction to Polymer Science,V.R.Gowarikar,N.V.Vishwanathan and J.Sridhar,Wiley Eastern.

DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER – II)

Paper No. : **IV (Code- MCH - 409)**
Compulsory /Optional : **Compulsory**
Max. Marks : **100**

Paper – IV : Spectroscopy II & Diffraction Methods

Unit – I	**Nuclear Magnetic Resonance Spectroscopy** Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant "j" Classification (AXB, AMX, ABC, A_2B_2 etc.). Spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton-^{13}C, ^{19}F and ^{31}P. FT NMR, advantages of FT NMR.
Unit – II	**Nuclear Quadrupole Resonance Spectroscopy** Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting. Applications.
Unit – III	**Electron Spin Resonance Spectroscopy** Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and Mc Connell relationship, measurement techniques, applications.
Unit – IV	**X-ray Diffraction** Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.
Unit –V	**Electron Diffraction** Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces. **Neutron Diffraction** Scattering of neutrons by solids measurement techniques, Elucidation of structure of magnetically ordered unit cells.

Books suggested:

1. Modern Spectroscopy, J.M. Hollas, John Viley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Inter science.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH- Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper &Row.

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M.Sc. CHEMISTRY (SEMESTER – II)

Paper No. : **V (Code- MCH - 410)**
Compulsory /Optional : **Compulsory**
Max. Marks : **100**

Paper – V : Computers For Chemists

This is a theory cum-laboratory co use with more emphasis on laboratory work.

Unit – I	**Introduction to computers and Computing** Basic structure and functioning of computer with a PC as illustrative example. Memory I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Principles of programming Algorithms and flow-charts.
Unit – II	**Computer Programming in FORTRAN/C/BASIC** (The language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C the features may be replaced appropriately). Elements of the compute language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Termination statements. Branching statements as IF or GO TO statement. LOGICAL variables. Double precession variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learns the programming logic and these language feature by hands on experience on a personal computer from the beginning of this topic.)
Unit – III	**Programming in Chemistry** Developing of small computer codes using any one of the languages FORTRAN/C/BASIC involving simple formulae in Chemistry, such as Vander Waals equation. Chemical kinetics (determination of Rate constant) Radioactive decay (Half Life and Average Life). Determination Normality, Molarity and Molality of solutions. Evaluation Electronegativity of atom and Lattice Energy from experimental determination of molecular weight and percentage of element organic compounds using data from experimental metal representation of molecules in terms of elementary structural features such as bond lengths, bond angles.
Unit – IV	**Use of Computer Programmes** Operation of PC. Data Processing. Running of standard Programs and Packages such as MS WORD, MS EXCEL -special emphasis on calculations and chart formations. X-Y plot. Simpson's Numerical Integration method. Programmes with data preferably from physical chemistry laboratory.
Unit –V	**Internet** Application of Internet for Chemistry with search engines, various types of files like PDF, JPG, RTF and Bitmap. Scanning, OMR, Web camera.

Books suggested:

1. Fundamentals of Computer : V. Rajaraman (Prentice Hall)
2. Computers in Chemistry : K.V. Raman (Tata Mc Graw Hill)
3. Computer Programming in FORTRAN IV-V Rajaraman (Prentice Hall)

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M. Sc. CHEMISTRY PRACTICALS (SEMESTER – II)

Practical examination shall be conducted separately for each branch : (Duration : 6-8 hrs in each branch).

Inorganic Chemistry

Chromatography		12
Preparations		12
Record		04
Viva-Voce		05
	Total :	33

Chromatography : Separation, identification & determination of cations & anions by Column Chromatography : Ion exchange.

Preparations : Preparation of selected inorganic complexes, their analysis, test & characterization by spectral techniques (may be).

(1) $K_3[Cr(SCN)_6].4H_2O$.
(2) $[Co(NH_3)_4(NO_2)_2]Cl$.
(3) $[Co(NH_3)_5Cl]Cl_2$.
(4) $Ni(dmg)_2$.
(5) $[Co(py)_2Cl_2]$.
(6) $[Cu.3[CS(NH_2)]_2SO_4.2H_2O$.
(7) $Na_3[Co(NO_2)_6]$.

Organic Chemistry

Organic Synthesis		12
Quantitative Analysis		12
Record		04
Viva-Voce		05
	Total :	33

Organic Synthesis :

(A) Synthesis involving name reactions :

(i) Sandmeyer's reaction.
(ii) Cannizaro's reaction.
(iii) Diel's Alder reaction.
(iv) Knoevenagel reaction.

(B) Synthesis of Dyes :

(i) Phenolphthalein, (ii) Fluoroscein, (iii) Diazotization followed by coupling.

Quantitative Estimations :

1. Determination of the percentage or number of hydroxyl groups in an organic compound by Acetylation method.
2. Estimation of amines / phenols using Bromate – Bromide solution or Acetylation method.
3. Saponification value, iodine value & acid values of an oil or fat.

Physical Chemistry

Any **one** Experiment / Exercise from **Section – A**		12
Any **one** Experiment / Exercise from **Section – B**		13
Record		04
Viva-Voce		05
	Total :	34

Section – A

Conductometry

(i) Determination of the velocity constant, order of the reaction & energy activation for saponification of ethyl acetate by sodium hydroxide conducotmetrically.

(ii) Determination of solubility & solubility product of sparingly soluble salts (e.g., $PbSO_4$, $BaSO_4$) conductometrically.

(iii) Determination of the strength of strong & weak acid in a given mixture conductometrically.

(iv) To study the effect of solvent on the conductance of $AgNO_3$ / acetic acid & to determine the degree of dissociation & equilibrium constant in different solvents & in their mixtures (DMSO, DMF, dioxane, acetone, water) & to test the validity of Debye – Huckel – Onsager theory.

(v) Determination of the activity coefficient of zinc ions in the solution of 0.002M zinc sulphate using Debye Huckel's limiting law.

Polarimetry

(i) Determination of rate constant for hydrolysis / inversion of sugar using a polarimeter.

(ii) Enzyme kinetics – inversion of sucrose.

Section – B

Potentiometry / pH metry

1. Determination of strengths of halides in a mixture potentiometrically.
2. Determination of the strengths of strong & weak acids in a given mixture using a Potentiometer / pH-meter.
3. Determination of temperature dependence of EMF of a cell.
4. Determination of the formation constant of silver – ammonia complex & stoichiometry of the complex Potentiometrically.
5. Acid – base titration in a non – aqueous media using a pH-meter.

Refractometry

Determination of Refractive indices & specific refractions, Molar & atomic refractivities, composition of a mixture of liquids, concentration of sugar in a solution & polarizabilities of liquids.

Books suggested

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly. Prentice Hall.
3. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall.
4. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Health.
5. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
6. Handbook of Organic Analysis-qualitative and Quantitative, H. Clark, Adward Arnold.
7. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
8. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
9. Findley's Practical Physical chemistry, B.P. Levitt, Longman.
10. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.