DEVI AHILYA VISHWAVIDYALAYA, INDORE

Scheme of Marks

M. Sc. Chemistry

(w.e.f. 2018 and onwards)

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

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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.

06/2/2018 6.2.18 6/2/18 6.2.18 06.02.18

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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.

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Unit –V	**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.

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M.Sc. CHEMISTRY (SEMESTER – II)

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

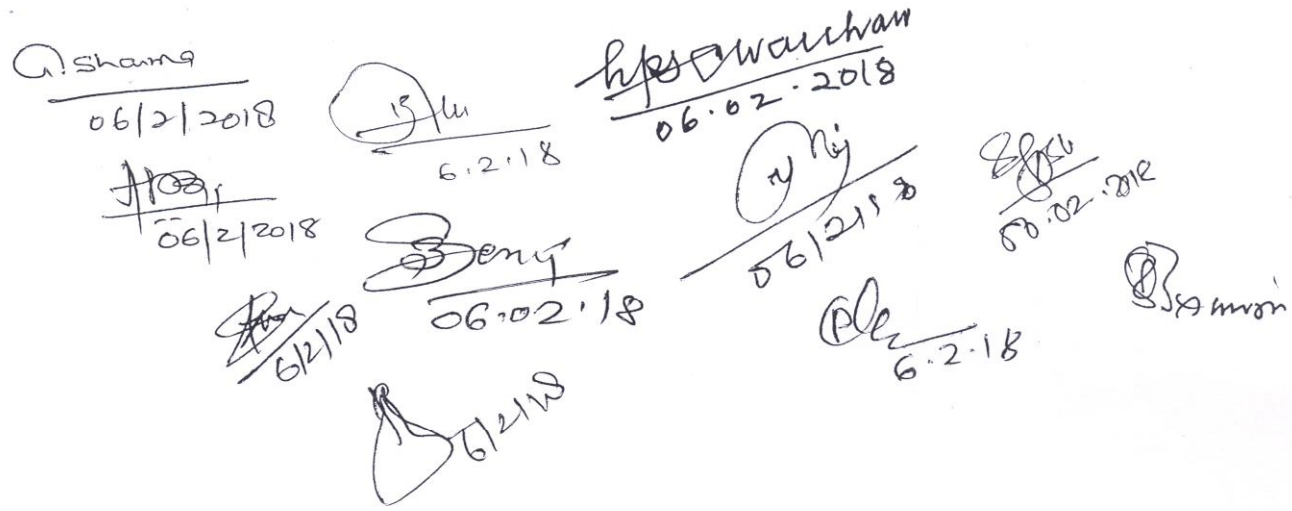
Paper – III : Physical Chemistry

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.

Unit –V	**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.



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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 course 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)

06.02.2018

DEVI AHILYA VISHWAVIDYALAYA, INDORE

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.