

# M.Sc. Chemistry I<sup>st</sup> Semester

Choice Based Credit system(CBCS)

Examination Session-2020-22

## Course Structure and Scheme

Course Code	Course Name	Total Marks	Credit	End Sem Exam Marks		Sessional Marks	
				MAX	MIN	MAX	MIN
MCH 101	Inorganic Chemistry-I	100	3	60	21	40	14
MCH 102	Organic Chemistry-I	100	3	60	21	40	14
MCH 103	Physical Chemistry-I	100	3	60	21	40	14
MCH 104	Group Theory & Spectroscopy-I	100	3	60	21	40	14
MCH 105	Practical-I (Inorganic Chemistry)	100	2	60	21	40	14
MCH 106	Practical-II (Organic Chemistry)	100	2	60	21	40	14
MCH 107	Practical-III (Physical Chemistry)	100	2	60	21	40	14
MCH 108	Seminar*	100	1	100	35	xx	xx
MCH 109	Assignment*	100	1	100	35	xx	xx
	<b>Sub Total</b>		20				
MCH 110	Comprehensive Viva*	100	4	100	35	xx	xx
	<b>Grand Total</b>		24				

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\* AE- Ability Enhancement / SD- Skill Development

SEMESTER-I

Paper-I

MCH-101: INORGANIC CHEMISTRY-I

Unit - I

**Stereochemistry and Bonding in Main Group Compounds:**

Valence shell electron pair repulsion (VSEPR) theory and its applications, bent Bonds,  $d\pi-p\pi$  bond, Bent rule, Some simple reactions of covalently bonded molecules such as Atomic inversion, Berry pseudo rotation, Nucleophilic displacement, free radical mechanisms.

Unit - II

**Metal Ligand bonding:**

Limitation of crystal field Theory, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes, symmetrically and asymmetrically filled  $t_{2g}$  and  $e_g$  sets of orbitals, Jahn -Teller effect, distortion in octahedral complexes ( $d^1-d^{10}$ ) metal ions, splitting of  $t_{2g}$  and  $e_g$  orbitals in elongated and compressed distorted octahedral complexes of  $Cu^{2+}$  ion.

Unit - III

**Metal -Ligand Equilibrium in Solution:**

Stepwise and over all formation constants and their relationship, 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 pH metry and Spectrometry.

## Unit - IV

### Reaction Mechanism of Transition Metal Complexes - I:

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 reaction in square planar complexes, the Trans effect, mechanism of substitution reactions.

## Unit-V

### Reaction Mechanism of Transition Metal Complexes - II and HSAB theory:

Redox reaction, Electron transfer reaction, mechanism of one electron transfer reaction, outer and inner sphere type reactions, cross reactions and Marcus - Hush theory, HSAB principle, Theoretical basis of hardness and softness, Lewis - acid base reactivity approximation; donor 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 Elements. N. N. Greenwood and A. Earnshaw, Pergamon
4. Inorganic Electronic Spectroscopy, A.B. P. Lever, Elsevier.
5. Comprehensive Co-ordination Chemistry eds., G. Wilkinson, R.D. Gillars and J. A. Mc Cleverty, Pergamon.
6. Inorganic Chemistry, D. F. Shriver & P.W. Atkins, Oxford University Press 3<sup>rd</sup> 1999.
7. Inorganic Chemistry by A.G.Sharpe. Addition Wesley England 3<sup>rd</sup> 1992
8. Inorganic Chemistry G.L.Misseler and D. A. Tarr Pearson Education, 2009.



## Paper-II

### MCH – 102: ORGANIC CHEMISTRY- I

#### Unit - I

##### **Nature of Bonding in Organic Molecules:**

Delocalized chemical bonding-conjugation and cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, anti-aromaticity and homo-aromaticity, PMO approach. Crown ether complexes.

#### Unit - II

##### **Stereochemistry:**

Elements of symmetry, Criteria for chirality, molecules with more than one chiral center, Threo and erythro isomers, Stereospecific and stereoselective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon biphenyls and allenes. Enantiomers and diastereomers. Methods of Resolution of racemic mixtures.

#### Unit - III

##### **Conformational analysis and linear free energy relationship:**

Conformational analysis of cyclohexane, decalines, effect of conformation on reactivity. Generation, structure, stability and reactivity of carbocation, 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:

Types of organic reactions and types of reactions and simple mechanism. Thermodynamic and kinetic requirements, Kinetic and thermodynamic control, Hammond's Postulate, Curtin-hammett principle. Potential energy diagrams, Transition states and intermediates, isotopic effects.

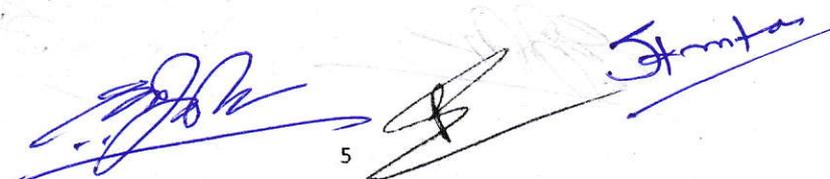
## Unit - V

### Aliphatic Nucleophilic Substitution:

The  $SN^2$ ,  $SN^1$ , mixed  $SN^1$  and  $SN^2$  and SEI mechanism. The neighboring group mechanism. Neighboring group participation by pi and sigma bonds, anchimeric assistance. Classical and non classical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. Nucleophilic substitution at an allylic. Effects of substrate structure, attacking nucleophiles, leaving group and reaction medium in  $SN^1$  &  $SN^2$  reactions.

### Book Suggested:

1. Advanced Organic Chemistry - Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell 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 & Professionals.
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.



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### Paper-III

## MCH - 103: PHYSICAL CHEMISTRY-I

### Unit - I

#### Introduction to Exact Quantum Mechanical Results :

Schrodinger 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.

### 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 calculation. Applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene etc.

### 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, antisymmetry 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 their quantities. Concepts of fugacity and determination of fugacity. 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 transition.

### Unit - V

#### Statistical Thermodynamics :

Concept of distribution, thermodynamics 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 thermodynamics probability in terms of partition. Application of partition functions. Fermi-Dirac Statistics, distribution law and application to metal. Bose-Einstein statistics distribution Law.

#### 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. Couison's Valence, R.Mc Weepy, ELBS.
5. Chemical Kinetic. K. J. Laidler, MoGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J. Rajaraman and J. Kuriacose, Mc Milian.
7. Micelies, 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 Bastern.
10. Introduction to Quamum Chemistry-R.K. Prasad New Age Publication.



## Paper-IV

### MCH – 104: Group Theory & Spectroscopy I

#### Unit – I

##### **Symmetry and Group theory in Chemistry:**

Symmetry elements and symmetry operation, definition of point group, subgroup. Schoenflies symbols, Conjugacy relation and classes., representations of groups by matrices (representation for the  $C_n, C_{nv}, C_{nh}$ , and  $D_{nh}$  group to be worked out explicitly) . 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

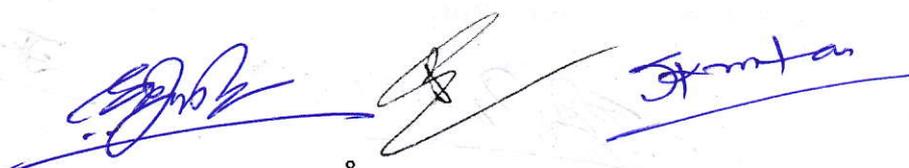
##### **Microwave Spectroscopy :**

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 vibration, normal co-ordination analysis.



## Unit - IV

### Raman Spectroscopy:

Classical and quantum theories of Raman effect. Vibration 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 transition, 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.

### Books suggested :

1. Modern Spectroscopy, I.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and FL. 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.



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**MCH-105: PRACTICAL (Inorganic Chemistry) Credit # 2**  
**(Duration: 6 - 8 hrs)**  
**External: 60, Sessional: 40**

**Inorganic Chemistry**

Quantitative / Qualitative Analysis	30
Preparation	12
Record	08
Viva Voice	10

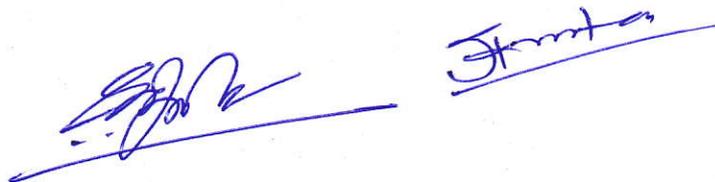
**Quantitative and Qualitative Analysis:**

- a. Less common metal ions: Ti, Mo, W, Zr, Th, V, U, ( two metal ions in cationic/anionic forms).
- b. Insoluble-Oxides, sulphates and halides.
- c. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc, involving volumetric and gravimethods.

**Preparations:**

Preparations of selected inorganic compounds and their studies by I.R. electronic spectra, Mossbauer, E.S.R. and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds.

1. VO(acac)<sub>2</sub>
2. TiO(C<sub>9</sub>H<sub>8</sub>NO)<sub>2</sub>H<sub>2</sub>O
3. Cis-K[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]
4. Na[Cr(NH<sub>3</sub>)<sub>2</sub>(SCN)<sub>4</sub>]
5. Ni(acac)<sub>2</sub>.
6. K<sub>3</sub>[Fe(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>]
7. Prussian Blue, Turnbull's Blue.



**MCH-106: Practical (Organic Chemistry) Credit # 2**  
**External: 60, Sessional: 40**

**Organic Chemistry**

Qualitative Analysis	21
Organic Synthesis	21
Record	08
Viva	10

**Qualitative Analysis:**

Separation, purification and identification of compounds of ternary mixture (one liquid and one solid) using TLC and column chromatography, chemical tests, IR spectra to be used for functional group identification.

**Organic Synthesis:**

Acetylation: Acetylation of Cholesterol and separation of cholesteryl acetate by column chromatography Oxidation: Adipic acid by chromic acid Oxidation of cyclohexanol. Grignard reaction: Synthesis of triphenyl menthanol from benzoic acid.

The products may be characterized by spectral techniques.



**MCH-107: Practical (Physical Chemistry) Credit # 2**  
**External: 60, Sessional: 40**

Adsorption and Phase Diagram	11
Chemical Kinetics	20
Solution	11
Record	08
Viva Voice	10

**Adsorption and Phase Diagram:**

Adsorption to study surface tension-concentration relationship for solutions (Gibbs Equilibria).

- i. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).
- ii. Determination of glass transition temperature of given salt (e.g.  $\text{CaCl}_2$ ) by conductometry.
- iii. To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water)

**Chemical Kinetics:**

- I. Determination of the effects of (a) Change of temperature, (b) Change of concentration of reactant and catalyst and (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 reactions.
- IV. Flowing clock reactions (Ref. Experiments in physical Chemistry by showmaker)
- V. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ions is oxidized by persulphate ion).
- VI. Oscillatory reaction.

**Solution:**

- I. Determination of molecular weight of non - volatile and electrolyte / electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
- II. Determination of degree of dissociation of weak electrolyte and to study the deviation from ideal behavior that occurs with a strong electrolyte.



# M.Sc. Chemistry 2<sup>nd</sup> Semester

Choice Based Credit system(CBCS)

Examination Session-2020-22

## Course Structure and Scheme

Course Code	Course Name	Total Marks	Credit	End Sem Exam Marks		Sessional Marks	
				MAX	MIN	MAX	MIN
MCH 201	Inorganic Chemistry-II	100	3	60	21	40	14
MCH 202	Organic Chemistry-II	100	3	60	21	40	14
MCH 203	Physical Chemistry-II	100	3	60	21	40	14
MCH 204	Group Theory & Spectroscopy-II	100	3	60	21	40	14
MCH 205	Practical-I (Inorganic Chemistry)	100	2	60	21	40	14
MCH 206	Practical-II (Organic Chemistry)	100	2	60	21	40	14
MCH 207	Practical-III (Physical Chemistry)	100	2	60	21	40	14
MCH 208	Seminar*	100	1	100	35	xx	xx
MCH 209	Assignment*	100	1	100	35	xx	xx
	<b>Sub Total</b>		20				
MCH 210	Comprehensive Viva*	100	4	100	35	xx	xx
	<b>Grand Total</b>		24				

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\* AE- Ability Enhancement / SD- Skill Development

## Semester - II

### MCH -201: Inorganic Chemistry- II

#### Unit - 1

##### Electronic Spectral Studies of Transition Metal Complexes:

Spectroscopic ground states, correlation between Orgal and Tanabe – Sugano diagrams for transition metal complexes ( $d^1$ -  $d^9$  states), Selection rules for electronic spectra. Intensity of various type electronic transitions. Calculation of  $Dq$ ,  $B$  and  $\beta$  parameters, charge transfer spectra.

#### Unit - 2

##### Magnetic Properties of Transition metal Complexes:

Type of magnetic bodies, two sources of paramagnetism, orbital and spin effect, Curie equation and Curie – wies law, Determination of magnetic susceptibility, Quenching of orbital contribution, Anomalous magnetic moment, Spin cross over and magnetic exchange coupling.

#### Unit- 3

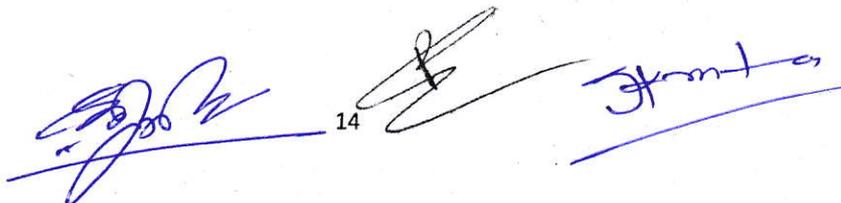
##### Metal $\pi$ Complexes:

Preparation, structure, bonding, and vibrational spectra of metal carbonyls and structure elucidation, important reaction of metal carbonyls, preparation, bonding, and structure of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligand.

#### Unit - 4

##### Metal Clusters:

Higher boranes, carboranes, metalloboranes and metallocarboranes compounds, dinuclear, trinuclear, tetranuclear, hexanuclear clusters with metal-metal multiple bonds.

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## Unit - 5

### Optical Rotatory Dispersion and Circular Dichroism:

Linearly and circularly polarized lights, optical rotator power and circular birefringence, Ellipticity and circular dichroism, ORD and Cotton effect, Faraday and Kerr effects, Assignment of electronic transitions, application of ORD and CD for the determination (i) absolute configuration of complexes and (ii) isomerism due to non planarity of chelate rings.

### Book Suggested

5. Advanced Inorganic Chemistry, F. A. Cotton and Wilkinson. JohnWiley.
6. Inorganic Chemistry, J. E. Huey, Harps and Row.
7. Chemistry of the element, N. N. Greenwood and A. Ernshow. Pergamon.
8. Inorganic Electronic Spectroscopy, A. B. P. LEVER, Elsevier.
9. Magnetochemistry, R. I. Carlin, Springer verlag.
10. Comprehensive Coordiantion Chemistry eds. G. Wilkinson, R. D. Gillars and J. A. Mc Cleverty, pergamon.
11. Element of magnetochemistry. A. Shyamal & R.L. Dutta.



# MCH – 202: ORGANIC CHEMISTRY- II

## Unit – I

### Aromatic Electrophilic Substitution:

The arenium ion mechanism, Nitration, Sulphonation, halogenation & Friedel craft reaction (alkylation and acylation) orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack. Diazonium coupling, Vilsmeier reaction, Gatterman - Koch reaction.

### Aromatic Nucleophilic Substitution:

The S<sub>N</sub>Ar and S<sub>N</sub>1, mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richter. Sommelet – Hauser, and Smiles rearrangements. Benzyne reaction and mechanism evidences in favour of benzyne reaction.

## Unit – II

### Free Radical Reactions:

Types of free radical reactions, free radical substitution mechanism, Reactivity for aliphatic and aromatic substrates at a bridgehead. The effect of solvents on reactivity. Allylic halogenations (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 and nucleophiles, Region – and chemoselectivity, Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

  
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## Unit – IV

### Addition to Carbon – Hetero Multiple bonds :

Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl compounds. Mechanism of condensation reactions involving enolates–Aldol, Knoevenagel, Claisen, Mannich, Benzoin & Perkin reaction.

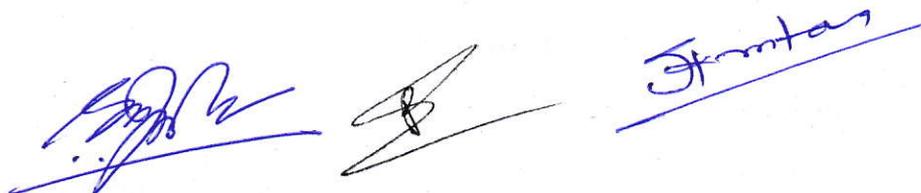
### Elimination Reactions:

The E2, E1 and E1cb reactions and their mechanism. Orientation of the double bond. Effects of substrate structures, attacking base and the leaving group on E-1, E-2 & E1cb reactions.

## Unit – V

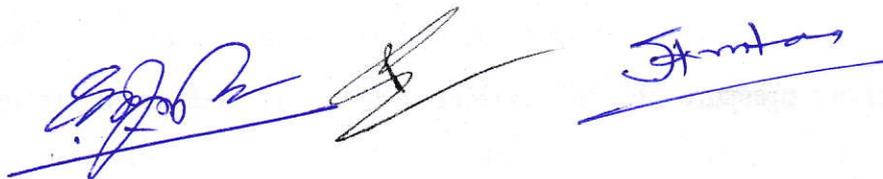
### Pericyclic Reactions:

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3- butadiene, 1, 3, 5,- hexatriene and allyl system. Classification of Pericyclic reaction. 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, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheletopic reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, 3,3-and 5,5 Sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Ene reaction.



**Book Suggested :-**

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



## MCH – 203: PHYSICAL CHEMISTRY- II

### Unit – I

#### Chemical Dynamics:

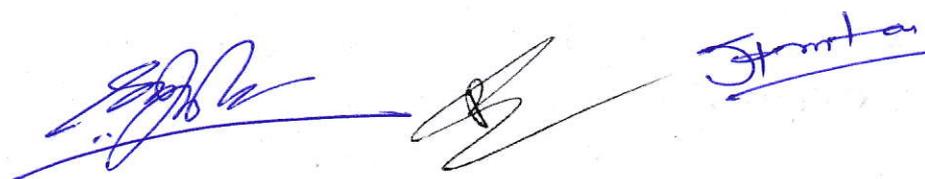
Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and activated complex theory: ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reaction, treatment of unimolecular reactions. 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 reaction (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 interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action model, solubilization, 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:

Thermodynamics criteria for non- Equilibrium state, entropy production and entropy flow, entropy balance equation 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 relation, 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 equation. Derivation of electro capillarity, Lippmann equations (surface excess). Methods of determination. Structure of electrified interfaces. Overpotential, exchange current density, derivation of Butler Volmer equation, Tafelplot. 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:**

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



## MCH – 204: Spectroscopy- II and 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, A2B2 etc ) spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton-<sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P FT NMR, advantages of FT NMR.

### Unit – II

#### 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 – III

#### X-ray Diffraction-I :

Generation of X-rays, X-ray tubes, Synchrotron source, Lattice, Planes, Miller indices, X-ray diffraction, Bragg's law, Reciprocal lattice, crystal symmetry, Space groups, Systematic absences, crystal growing, Screening and mounting, Data collection, Data reduction, Theory of Structure factors and Fourier Synthesis, Phase problem and its solution, Structure solution and refinement.



## Unit – IV

### **X-ray Diffraction-II:**

Derivation of X-rays results, determination of absolute configuration of the molecules, Overview of important crystallographic programmes, random and Systematic errors, File structure for SHELXL and its commands, Diagrams, tables, Use of XP, Structure Validation, Disorder, Types of disorder and their solution, solvent disorder, twining, Types of twining and their solution, Crystallographic database.

## Unit – V

### **Electron Diffraction:**

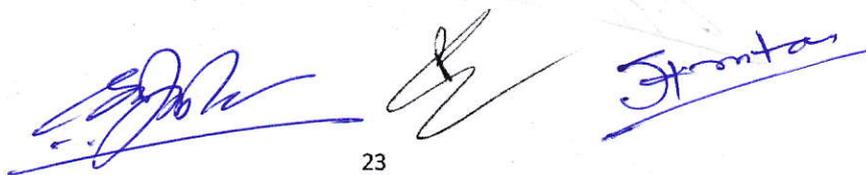
Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

### **Neutron Diffraction:**

Scattering of neutrons by solids measurement techniques, Elucidation of structure of magnetically ordered unit cells.

### **Books suggested**

11. Modern Spectroscopy, J.M. Hollas, John Viley.
12. Applied Electron Spectroscopy for chemical analysis D. H. Windawi and F.L.Ho, Wiley Interscience.
13. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic chemistry, R. V. Parish, Ellis Harwood.
14. Physical Methods in Chemistry, R. S. Drago, Saunders College.
15. Chemical Applications of Group theory, F. A. Cotton.
16. Introduction to Molecular Spectroscopy, G. M. Barrow, Mc Graw Hill.



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17. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
18. Theory and Application of UV Spectroscopy, H. H Jaffe and M. Orchin, IBH Oxford.
19. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
20. Introduction to Magnetic Resonance. A. Carrington and A. D. Maclachalan, harper & Row.

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**MCH-205: PRACTICAL (Inorganic Chemistry) CREDIT # 2**

**External: 60, Sessional: 40**

Chromatography	21
Preparation	21
Record	08
Viva Voice	10

**Chromatography:**

Separation of cations and anions by paper chromatography / column chromatography (ion exchange).

**Preparations:**

Preparation of selected inorganic compounds and their students by I. R. electronic spectra, Mossbauer, E.S.R. and magnetic susceptibility measurements. Handling of air and moisture compounds.

1.  $[\text{Co}(\text{NH}_3)_6] [\text{Co}(\text{NO}_2)_6]$
2. Cis- $[\text{Co}(\text{trien})(\text{NO}_2)_2] \text{Cl} \cdot \text{H}_2\text{O}$
3. Hg  $[\text{Co}(\text{SCN})_4]$
4.  $[\text{Co}(\text{Py})_2 \text{Cl}_2]$
5.  $[\text{Ni}(\text{NH}_3)_6] \text{Cl}_2$
6. Ni (dmg)<sub>2</sub>
7.  $[\text{Cu}(\text{NH}_3)_4] \text{SO}_4 \cdot \text{H}_2\text{O}$



**MCH-206: PRACTICAL (Organic Chemistry) CREDIT # 2**

**External: 60, Sessional: 40**

Organic Synthesis	21
Qualitative Analysis	21
Record	08
Viva	10

**Organic Synthesis:**

Aldol condensation, dibenzal acetone from benzaldehyde, sandmeyer reaction: p-chlorotoulene from p-toluidine. Acetoacetic ester condensation: synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation, Cannizzaro reaction: 4-chloro benzaldehyde as substrate. Friedel crafts reaction:  $\beta$ -Benzoyl propanoic acid from succinic anhydride and benzene. Aromatic electrophilic substitutions: Synthesis of p-nitroaniline and p-bromoaniline. The products may be characterized by Spectral Techniques.

**Qualitative Analysis:**

Determination of the percentage or number of hydroxyl group in an organic compound by acetylation method. Estimation of amines/phenols using brominated solution/or acetylation method. Determination of iodine saponification values of an oil sample.



## MCH-207: PRACTICAL (Physical Chemistry) CREDIT # 2

External: 60, Sessional: 40

Conductometry	16
Potentiometry/pH metry	16
Polarimetry	10
Record	08
Viva voce	10

### Conductometry:

- Determination of the velocity constant, order the reaction energy of activation saponification of ethyl acetate by sodium hydroxide conductometrically.
- Determination of solubility product of sparingly soluble salts,  $PbSO_4$ ,  $BaSO_4$  conductometrically.
- Determination of the strength of strong and weak acid in a given mixture conductometrically.
- to study of the effect of solvent on the conductance of Ag No 3/acetic acid to determine the degree of dissociation equilibrium constant in different solvents in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
- Determination of the activity coefficient of zinc ions in the solution 0.002M zinc sulphate using Debye Huckel's limiting law.

### Potentiometry/pH metry:

- Determination of strengths of halides in a mixture potentiometrically.
- Determination of the valency of mercurous ions potentiometrically.
- Determination of the strength strong and weak acids in a given mixture using a potentiometer/pH meter.
- Determination of temperature dependence EMF of a cell.
- Determination of formation constant silver ammonia complex and stoichiometry of the complex potentiometrically.
- Acid – base titration in a non – aqueous media using a pH meter.
- Determination of activity and activity coefficient of electrolytes.
- Determination of the dissociation constant of acetic acid in DMSO. DMF, acetone, dioxane by titrating it with KOH.
- Determination of the dissociation constant of monobasic / dibasic acid by Albert – Sderjeant method.
- Determination of thermodynamic constants,  $D_g$ ,  $D_S$ , and  $D_H$  for the reaction by e. m. f. method.  $Zn + H_2SO_4 > ZnSO_4 + H_2$

### Polarimetry:

- Determination of rate of constant for hydrolysis / inversion of sugar using a polarimeter.
- Enzyme kinetics-inversion of sucrose.



**M.Sc. Chemistry Third Semester**  
**Choice Based Credit system(CBCS)**  
**Examination Session-2020-22**  
**Course Structure & Scheme**

Course Code	Course Name	Total Marks	Credit	End Sem Exam Marks		Sessional Marks	
				MAX	MIN	MAX	MIN
MCH 301	Application of Spectroscopy (Inorganic Chemistry)	100	3	60	21	40	14
MCH 302	Photochemistry	100	3	60	21	40	14
MCH 303	Analytical Chemistry	100	3	60	21	40	14
MCH 304	Medicinal Chemistry	100	3	60	21	40	14
MCH 305	Practical-I (Inorganic Chemistry)	100	2	60	21	40	14
MCH 306	Practical-II (Organic Chemistry)	100	2	60	21	40	14
MCH 307	Practical-III (Physical Chemistry)	100	2	60	21	40	14
MCH 308	Seminar*	100	1	100	35	xx	xx
MCH 309	Assignment*	100	1	100	35	xx	xx
	<b>Sub Total</b>		20				
MCH 310	Comprehensive Viva*	100	4	100	35	xx	xx
	<b>Grand Total</b>		24				




\* AE - Ability Enhancement / SD - Skill Development

## SEMESTER III

### MCH – 301: Application of Spectroscopy

#### (Inorganic Chemistry)

##### Unit – I

###### **Electronic Spectra of coordination compounds:**

Electronic transition selection rule, selection rule and d-d transition in metal complexes, Effect of spin-orbit coupling, spin forbidden transitions. Band contours and band intensities, Jahn Teller distortion and spectra, Electronic spectra of  $d^1$ - $d^9$  system in octahedral and tetrahedral complexes, Applications of Tanabe-Sugano diagram for determination of  $10 Dq$  ( $\Delta_o$ ) from spectra, Charge transfer spectra in metal complexes.

##### Unit – II

###### **Vibrational Spectroscopy:**

Symmetry and shapes of  $AB_2$ ,  $AB_3$ ,  $AB_4$ ,  $AB_5$ ,  $AB_6$  mode of bonding of ambidentate ligands, nitrosyl, ethylenediamine and diketonato complexes, application of resonance Raman Spectroscopy particularly for the study of active sites of metalloproteins.

##### Unit – III

###### **Electron Spin Resonance Spectroscopy:**

Hyperfine coupling, Spin polarization for atoms and transition metal ions. Spin - orbit coupling and significance of g- tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals.



## Unit – IV

### Application of Nuclear Magnetic Resonance in coordination compounds:

Applications of NMR spectroscopy to co-ordination compounds (based on chemical shift and coupling constant) using examples of metal nuclide  $^{77}\text{Se}$ ,  $^{113}\text{Cd}$ ,  $^{119}\text{Sn}$ ,  $^{125}\text{Te}$ ,  $^{195}\text{Pt}$ ,  $^{199}\text{Hg}$ , Contrast agents, Shift reagent.

## Unit - V

### Mossbauer Spectroscopy:

Basic principle, Mossbauer nuclides and their characteristics, instrumentation, chemical shift, , Quadrupole effect, Magnetic field effect, Application of the technique to studies of (1) bonding and structure of  $\text{Fe}^{+2}$  and  $\text{Fe}^{+3}$  Compounds (2) detection of oxidation state in  $\text{Sn}^{+2}$  and  $\text{Sn}^{+4}$  compounds .

### BOOKS SUGGESTED:

- 2 Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
- 3 Infrared and Raman Spectral Inorganic and Co-ordination compounds K. Nakamalo, Wiley.
- 4 Progress in Inorganic Chemistry vol. 8, ed. F.A. Cotton. Vol. 15 ed. S. J. Lippard, Wiley.
- 5 Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
- 6 NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.
- 7 Practical NMR Spectroscopy, M.L. Martin. J. J. Deepish and G. J. Martin, Heyden.
- 8 Application of Spectroscopy of Organic Compounds, J. R. Dyer Prentice Hall.
- 9 Spectroscopic Methods in Organic Chemistry D.H. Williams, I. Fleming, Tata Mc Graw - Hill.
9. Coordination compounds by S.F.A Kettle.
10. Inorganic Chemistry by G.L Miessler and D.A. Tarr

# MCH - 302: PHOTOCHEMISTRY

## Unit-I

### Photochemical Reactions:

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

## Unit - II

### Determination of Reaction Mechanism:

Classification, rate constants and life times of reactive energy state determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions-photo dissociation, gas-phase photolysis.

## Unit - III

### Photochemistry of Alkene :

Intramolecular reactions of olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1, 4 - and 1, 5 -dienes.

### Photochemistry of Aromatic Compounds:

Isomerisation, addition and substitution.

## Unit - IV

### Photochemistry of Carbonyl Compounds:

Intermolecular reactions of Carbonyl Compounds-saturated, cyclic and acyclic,  $\alpha, \beta$  unsaturated and  $\alpha, \gamma$  unsaturated Compounds, cyclohexadienones. Intermolecular cycloaddition reaction - dimerisations and oxetane formation.



## Unit - V

### Miscellaneous Photochemical Reactions:

Photo-Fries reaction of annelid's, Photo-Fries rearrangement. Barton reaction. Singlet molecular Oxygen reaction. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

### Books Suggested:

12. Fundamentals of photochemistry, K. K. Rothagi - Mukherji, Wiley - Eastern.
6. Essentials of Molecular Photochemistry, A Gilbert and J. Baggott, Blackwell Scientific Publication.
7. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
8. Introductory Photochemistry, A. Cox and t. Camp, McGraw Hill
7. Photochemistry, R. P. Kundall and A. Gilbert. Thomson Nelson.
8. Organic Photochemistry, J. Coxon and B. halton, Cambridge University Press.



## MCH – 303: Analytical Chemistry

### Unit – I

#### Introduction:

Role of analytical chemistry classification of analytical methods classical and instrumental. Types of instrumental analysis Selecting an analytical method Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware cleaning and Calibration of glassware. Sample preparation, dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

#### Errors and Evaluation:

Definition of terms in mean and median, Precision - standard deviation, relative standard deviation Accuracy - absolute error, relative error, Types of error in experimental data determinate (systematic), indeterminate (or random) and gross. Sources of error and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data - indeterminate errors. The uses of statistics.

### Unit II

#### Food Analysis:

Moisture, ash, crude protein, fat crude fiber, carbohydrates, calcium, potassium, sodium and phosphate food adulteration common. adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC Gas chromatography for organophosphates. Thin - layer chromatography for identification of chlorinated pesticides in food products.

### Unit-III

#### **Analysis of Water Pollution:**

Origin of Waste water, types, water pollutants and their effects. Sources of water pollution - domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis -parameter for analysis - colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen, Heavy metal pollution- public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD, and COD. Pesticides as water pollutants and analysis. Water Pollution laws and standards.

### Unit - IV

#### **Analysis of soil, Fuel, Body Fluids and Drugs:**

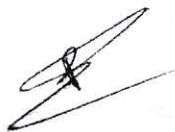
(a) Analysis of soil, moisture pH total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

(b) Fuel analysis : liquid and gas. Ultimate and proximate analysis-heating values-grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-produced gas and water gas-calorific value.

### Unit - V

#### **Clinical Chemistry:**

Composition of blood-collection and preservation of sample. Clinical analysis. Serum electrolytes, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphates. Immunoassay : principles of radio immunoassay (RIA) and applications. The blood gas analysis trace elements in the body.

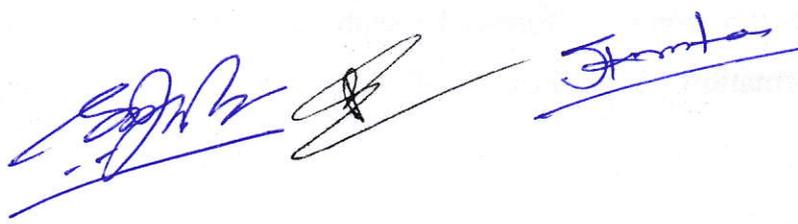


**Drug Analysis:**

Narcotics and dangerous drug. Classification of drugs. Screening by gas thin-layer chromatography and spectrophotometric measurements.

**Books Suggested:**

21. Analysis Chemistry, G.D. Christian, J. Wiley.
22. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Hooler, W.B. Sanuders.
23. Analysis Chemistry-Principles. J.H. Kennedy. W.B. Sanuders.



# MCH – 304: Medicinal Chemistry

## Unit - I

### Structure and Activity:

Relationship between chemical structure and biological activity (SAR). Receptor Site Theory Approaches to drug design. Factors affecting bioactivity. QSAR-Free-Wilson analysis, Hansch analysis, relationship between Free - Wilson analysis and Hansch analysis.

## Unit - II

### Pharmacodynamics:

Introduction, elementary treatment of enzymes stimulation and enzyme inhibition, Classification and mode of action of sulfonamides with examples, Drug metabolism, xenobiotics, biotransformation. Significance of drug metabolism in medicinal chemistry.

## Unit - III

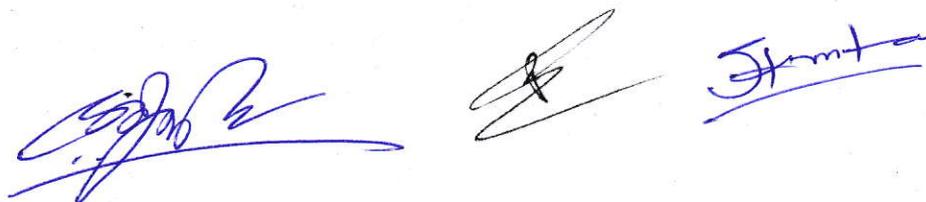
### Antibiotics and Antibacterial:

Introduction, Classification and mode of  $\beta$  -lactam type antibiotics, Antituberculars - Streptomycin, Broad spectrum antibiotic – Tetracyclines, Anticancer Drug-Dactinomycin.

## Unit - IV

General chemistry and mode of action of common Antifungal, Antibacterial and Antiviral drugs

Antimalarials: Chemotherapy of malaria. Chloroquine, Chlorquanide and Mefloquine.



## Unit - V

General chemistry, classification and mode of action of Non - steroidal Anti - inflammatory drugs: Diclofenac Sodium and Ibuprofen.

Anti-histamic and anti-asthmatic agents : Terfenadine, Cinnarizine and Salbutamol.

### Books Suggested:

1. Essentials of Medical Pharmacology, K.D.Tripathi
2. Medicinal Chemistry, Ashutosh Kar
3. Foye's principle's of Medicinal Chemistry, Williams and Lemke
4. Burger's Medicinal Chemistry and drug discovery



**MCH-305: PRACTICAL (INORGANIC CHEMISTRY) CREDIT # 2**

**External: 60, Sessional: 40**

**INORGANIC CHEMISTRY**

Quantitative determination of a three component mixture	21
Chromatographic Separations	21
Record	08
Viva voce	10

**Quantitative determination of a three component:**

One volumetrically and two gravimetrically

- (a)  $\text{Cu}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Zn}^{2+}$ .
- (b)  $\text{Cu}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Mg}^{2+}$ .

**Chromatographic Separations:**

- (a) Cadmium and Zinc.
- (b) Zinc and Magnesium.
- (c) Thin-layer chromatography-separation of Nickel, Manganese, Cobalt and Zinc.  
Determination of  $R_f$  values.

Separation and identification of sugar present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of  $R_f$  values.

## MCH-306: PRACTICAL (ORGANIC CHEMISTRY) CREDIT # 2

External: 60, Sessional: 40

Multi-step synthesis of organic compounds	21
Paper Chromatography	21
Record	08
Viva voice	10

### Multi-step synthesis of organic compounds:

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

1. Photochemical reaction Benzophenone  $\rightarrow$  Benzpinacol  $\rightarrow$  Benzpinacolone  
Beckmann rearrangement: Benzanilide from benzene Benzene  $\rightarrow$  Benzophenone  
 $\rightarrow$  Benzophenone oxime  $\rightarrow$  Benzanilide Benzilic acid rearrangement: Benzilic acid from benzoin Benzoin  $\rightarrow$  Benzil  $\rightarrow$  Benzilic acid
2. Synthesis of heterocyclic compounds Skraup synthesis: Preparation of quinoline from aniline. Fisher Indole synthesis: Preparation of 2-phenylindole from phenylhydrazine. Enzymatic synthesis Enzymatic reeducation: reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S (+) ethyl -3-hydroxybutanoate and determine its optical purity.
3. Biosynthesis of ethanol from sucrose. Synthesis using microwave Alkylation of diethyl malonate with benzyl chloride. Synthesis using phase transfer catalyst. Alkylation of diethyl malonate or ethyl acetoacetate with an alkylhalide.

### Paper Chromatography:

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R<sub>f</sub> values.



**MCH-307: PRACTICAL (Physical CHEMISTRY) CREDIT # 2**

**External: 60, Sessional: 40**

Spectroscopy	22
Chemical Kinetics	20
Record	08
Viva voice	10

**Spectroscopy:**

- (I) Determination of PKa of indicator (e.g. methyl red) in (a) aqueous and (b) micellae media.
- (II) Determination of stoichiometry and stability constant of Ferric isothiocyanate complex ion solution.
- (III) Determination of rate constant of alkaline bleaching of Malachite green and effects of ionic strength on the rate of reaction.

**Chemical kinetics:**

- (I) Determination of rate constant and formation constant of an intermediate complex in the reaction of Ce(IV) and Hypophosphorous acid at ambient temperature.
- (II) Determination of energy and enthalpy of activation in the reaction of  $\text{KMnO}_4$  and benzyl alcohol in acid medium.
- (III) Determination of energy of activation of and entropy of activation from a single kinetic run.
- (IV) Kinetics of an enzyme catalyzed reaction.



# M.Sc. Chemistry 4<sup>th</sup> Semester

Choice Based Credit system(CBCS)

Examination Session-2020-22

## Course Structure & Scheme

Course Code	Course Name	Total Marks	Credit	End Sem Exam Marks		Sessional Marks	
				MAX	MIN	MAX	MIN
MCH 401	Application of Spectroscopy (Organic Chemistry)	100	3	60	21	40	14
MCH 402	Solid State Chemistry	100	3	60	21	40	14
MCH 403	Organotransition Metal Chemistry	100	3	60	21	40	14
MCH 404	Polymer Chemistry	100	3	60	21	40	14
MCH 405	Practical-I (Inorganic Chemistry)	100	2	60	21	40	14
MCH 406	Practical-II (Organic Chemistry)	100	2	60	21	40	14
MCH 407	Practical-III (Physical Chemistry)	100	2	60	21	40	14
MCH 408	Seminar*	100	1	100	35	xx	xx
MCH 409	Assignment*	100	1	100	35	xx	xx
	<b>Sub Total</b>		20				
MCH 410	Comprehensive Viva*	100	4	100	35	xx	xx
	<b>Grand Total</b>		24				

\* AE - Ability Enhancement / SD - Skill Development

## SEMESTER IV

### MCH-401: APPLICATION OF SPECTROSCOPY

#### (Organic Chemistry)

#### Unit – I

##### Ultraviolet and visible spectroscopy:

Various electronic transitions Beer-Lambert law, effect of solvents on electronic transitions, Fieser Woodward rules for Conjugated dienes, ultraviolet spectra of aromatic compounds. Chromophore and auxochrome concepts, Effect of conjugation on  $\lambda_{\max}$ , allowed and forbidden transitions.

#### Unit – II

##### Infrared Spectroscopy:

Basic theory, spectrum, Modes of molecular vibrations. vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids and anhydrides,). Effect of hydrogen bonding and solvent on Carbonyl vibrational frequencies, intra molecular factors affecting the carbonyl absorption, overtones, combination bands and Fermi resonance.

#### Unit - III

##### Nuclear Magnetic Resonance Spectroscopy:

General introduction and definition, chemical shift, spin - spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon ( aliphatic, olefinic, aldehydic and aromatic ) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto ) chemical exchange, effect of deuteration, complex spin -



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spin interaction between two, three, four and five nuclei ( first order spectra ), Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with disordered angle.

Simplification of complex spectra, nuclear magnetic double resonance, NMR shifts reagents, solvent effect. Fourier transforms technique.

#### Unit – IV

##### Carbon-<sup>13</sup>NMR Spectroscopy:

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy – COSY, NOESY, DEPT, and INADEQUATE techniques.

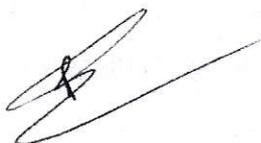
#### Unit – V

##### Mass spectrometry:

Introduction, ion production, FAB, factors affecting fragmentation, ion analysis, ion abundance Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak. Mc Lafferty rearrangement. Ortho effect, Retro-Diels-Alder reaction, homolytic and heterolytic cleavage, Hydrogen transfer reaction, Nitrogen rule. High resolution mass spectrometry.

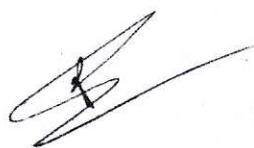
##### Book Suggested:

1. Physical Methods for chemistry, R . S. Drago, Saunders company.
2. Structural Methods in Inorganic chemistry, E.A.V. Ebswoth, D.W.H. Rankin and S. Cradock, ELBS.



3. Infrared and Raman spectral: Inorganic and Cordination Compounds K. Nakamoto, Wiley.
4. Progress in Inorganic chemistry vol., 8,ed., F.A. Cotton, vol., 15 ed. S. J. Lippard, Wiley.
5. Transition Metal chemistry ed. R.L. Carlin vol. 3 dekker.
6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.

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A handwritten signature in blue ink, possibly reading "R. L. Carlin", with a horizontal line underneath.

A handwritten signature in blue ink, possibly reading "A. P. B. Lever", with a horizontal line underneath.

# MCH-402: SOLID STATE CHEMISTRY

## Unit – I

### **Solid State Reactions:**

General principles, experimental procedure, co- precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

## Unit-II

### **Crystal Defects and Non- Stoichiometry:**

Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects. Vacancies-Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defects formation, colour centers, non-stoichiometry and defects.

## Unit-III

### **Electronic properties and Band Theory:**

Metal insulators and semiconductors, electronic structure of solids band theory band structure of Metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions,. Optical properties- Application of optical electron microscopy. Magnetic Properties-classification of materials : Effect of temperature calculation of Magnetic moment.

## Unit-IV

### **Organic Solids:**

Electrically conducting solids. Organic charge transfer complex, Organic metals, super conductors, types and applications, new super conductors.



## Unit-V

### Liquid crystals:

Types of liquid crystals: Nematic, Smectic, Ferroelectric, Anti-Ferroelectric,  
Various theories of LC, Liquid crystal display, new materials.

### Books Suggested:

1. Solid state chemistry and its application, A.R. West. Peenum.
2. Principals of Solid State, H.V. Keer, Wiley Eastern.
3. Solid state chemistry, N.B. Hannay.
4. Solid state chemistry, D.K. Chakrabarty, New Wiley Easte.



Skritas

# MCH-403: ORGANOTRANSITION METAL CHEMISTRY

## Unit - I

### Alkyls and Aryls of Transition Metals:

Type, routes of synthesis, stability and decomposition pathway, use of organocopper in organic synthesis.

### Compounds of Transition Metal-Carbon multiple bonds:

Alkylidenes, alkylidyne, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions of the ligands, role in organic synthesis.

## Unit - II

### Transition Metal $\pi$ - Complexes:

Transition Metal  $\pi$  - Complexes with unsaturated organic molecules such as alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparation, properties, nature of bonding and structural features. Important reaction relating to nucleophilic and electrophilic attack on ligands role in organic synthesis.

## Unit - III

### Stoichiometric reactions and Transition Metal Compounds with bonds to hydrogen, boron, silicon:

Stoichiometric reactions of main group organometallics such as organolithium, organosodium, organomagnesium, organozinc, organocadmium, organomercury,



organoaluminium, organothallium and organosilicon, transition metal compounds with bonds to hydrogen, boron, silicon.

## Unit – IV

### Homogeneous Catalysis:

Catalytic processes such as oxidative addition, insertion, elimination, polymer supported catalyst, homogeneous catalytic hydrogenation, Ziegler-Natta polymerization of olefins, hydroformylation of alkenes (oxo process), oxidation of alkenes, acetic acid synthesis and homologation of acetic acid.

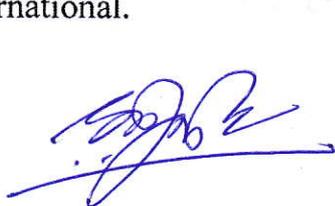
## Unit-V

### Fluxional Organometallic Compounds:

Fluxionality and dynamic equilibrium in compounds such as acyclic alkenes,  $\sigma$ -bonded cyclic alkenes,  $\pi$ -bonded cyclic alkenes and metal carbonyls.

### BOOKS SUGGESTED:

20. Principles and Application of Organotransition Metal chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
21. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree John Wiley.
22. Metallo-Organic Chemistry, A.J. Pearson, Wiley.
23. Organometallic Chemistry, R.C. Mehrotra and A. Singh New age International.



# MCH-404 :POLYMER

## Unit – I

### Basics:

Importance of polymers. Basic concepts : Monomers, repeat units, degree of polymerization Linear, branched and network polymers. Classification of polymers. Polymerization : condensation, addition/radical chain-ionic and coordination and copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

## Unit – II

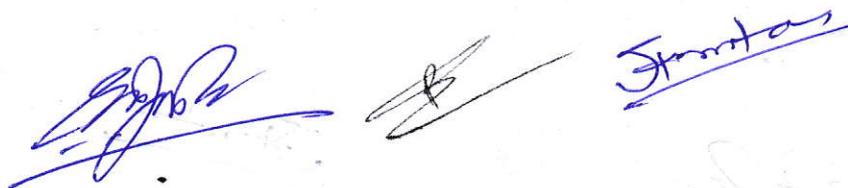
### Polymer Characterization:

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersion molecular weight distribution. The practical significance of molecular weight. End-group, Viscosity, light scattering, osmotic and ultracentrifugation methods.

## Unit – III

### Analysis and testing of Polymers:

Chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy . Thermal analysis and physical testing-tensile strength. Fatigue impact. Tear resistance, Hardness and abrasion resistance.



## Unit – IV

### Inorganic Polymers

Structure, Properties and Applications of

- a. Polymers based on boron-boranes and carboranes.
- b. Polymers based on Silicon, silicone's polymetalloxanes and polymetallosiloxanes, silazanes.

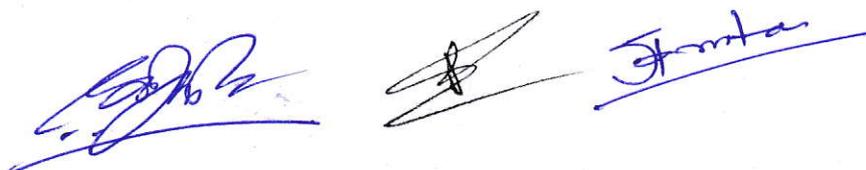
## Unit – V

Structure, Properties and Applications of

- a. Polymers based on Phosphorous, Phosphazenes, Polyphosphates.
- b. Polymers based on Sulphur-Tetrasulphur tetranitride and related compounds.
- c. Co-ordination and metal chelate Polymers.

### Books Suggested

24. Inorganic Chemistry, J.E. Huheey, Harper Row.
25. Developments in Inorganic polymers Chemistry, M.F. Lappert and G.J. Leigh.
26. Inorganic polymers – N.H. Ray.
27. Inorganic polymers, Graham and Stone.
28. Inorganic Rings and Cages : D.A. Armitage.
29. Textbook of Polymers Science, F.W. Billmeyer Jr. Wiley.
30. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.



**MCH-405: PRACTICAL (Inorganic Chemistry) Credit # 2**

**(Duration: 6 - 8 hrs)**

**External: 60, Sessional: 40**

Preparation	21
Spectrophotometric determinations	21
Record	08
Viva voce	10

**Preparation:**

Preparation of selected inorganic compounds and their studies by IR, electronic spectra and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines. Selection can be made from the following:

1. Sodium amide. Inorg. Synth., 1946, 2, 128.
2. Atomic absorption analysis of Mg and Ca.
3. Synthesis of trichlorodiphenylantimony (V) hydrate. Inorg. Synth., 1985, 23, 194
4. Sodium tetrathionate  $\text{Na}_2\text{S}_4\text{O}_6$ .
5. Metal complex of dimethyl sulfoxide:  $\text{CuCl}_2 \cdot 2\text{DMSO}$  J. Chem. Educ., 1982, 59, 57.
6. Synthesis of metal acetylacetonate: Inorg. Synths, 1957, 5, 130, 1963, 1, 183.
7. Cis and Trans  $[\text{Co}(\text{en})_2\text{Cl}_2]^+$ .
8. Determination of Cr (III) complex.  $[\text{Cr}(\text{H}_2\text{O})_6] \text{NO}_3 \cdot 3\text{H}_2\text{O}$ . Inorg. Synths., 1972, 13, 184.
9. Preparation and use of Ferrocene. J. Chem. Edu. 1966, 43, 73, 1976, 53, 730.
10. Preparation of  $[\text{Co}(\text{phenanthroline-5,6 quinone})]$ .

**Spectrophotometric Determination**

- a) Manganese/Chromium in steel sample.
- b) Nickel by extractive Spectrophotometric method.
- c) Fluoride/nitrite/phosphate.
- d) Copper-Ethylene diamine complex: Slope-ratio method.



**MCH-406: PRACTICAL (Organic Chemistry) Credit # 2**  
**(Duration: 6 - 8 hrs)**  
**External: 60, Sessional: 40**

Extraction of organic compounds from natural sources	21
Spectrophotometric Determination	21
Record	08
Viva voice	10

**Extraction of organic compounds from natural sources**

1. Isolation of caffeine from tea leaves.
2. Isolation of casein from milk (students are required to try some typical color reaction of protein).
3. Isolation of Lactose from milk (purity of sugar should be checked by LC and PC and RF values reported).
4. Isolation of nicotine diorite from tobacco.
5. Isolation of piperdine from black pepper.
6. Isolation of Lycopene from tomato.
7. Isolation of  $\beta$ -carotene from carrots.
8. Isolation of eugenol from clove.
9. Isolation of (+) Limonene from clove.

**Spectroscopy**

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS) Spectrophotometric (UV/VIS ) Estimations.

- 1). Amino acids
- 2). Proteins
- 3). Carbohydrates
- 4). Ascorbic acid
- 5). Aspirin
- 6). Caffeine



**MCH-407: PRACTICAL (Physical Chemistry) Credit # 2**

**(Duration: 6 - 8 hrs)**

**External: 60, Sessional: 40**

Thermodynamics	21
Polarography	21
Record	08
Viva voce	10

**Thermodynamics**

- i. Determination of partial molar volume of solute (e.g. KCL) and solvent in a binary mixture.
- ii. Determination of the temperature dependence of the solubility of a compound in two solvent having similar intramolecular interactions (Benzoic acid in water and in DMSO water mixture and calculate the partial molar heat of solution).

**Polarography**

- i. Identification and estimation of metal ions such as  $\text{Cd}^{+2}$ ,  $\text{Pb}^{+2}$ ,  $\text{Zn}^{+2}$  and  $\text{i}^{+2}$  etc. polarographically.
- ii. Study of metal ligand complex polarographically. (using Lingane's Method).

