

# **GONDWANA UNIVERSITY, GADCHIROLI**



## **Syllabus**

**for**

**Master of Science (M.Sc.) Chemistry**

**Based on NEP – 2020**

(with effect from 2023-24)

**Board of Studies in Chemistry**

**Faculty: Science and Technology**

**GONDWANA UNIVERSITY, GADCHIROLI**

**M.Sc.-I Semester I, II (Chemistry)**

**(NEP 2020, Effective from 2023-24)**

**M.Sc. (Chemistry)**

Scheme of Teaching and Examination for M.Sc. (Chemistry)									
M.Sc. (Chemistry) Semester – I									
	Subjects	L	T	P	Total Credits	UA	CA	Min	Total
<b>Major</b>	<b>01MSCCH01</b> Paper I (Inorganic Chemistry)	3	--	--	3	80	20	40	100
	<b>01MSCCH02</b> Paper II (Organic Chemistry)	3	--	--	3	80	20	40	100
	<b>01MSCCH03</b> Paper III (Physical Chemistry)	3	--	--	3	80	20	40	100
<b>Major Elective</b>	<b>01MSCCH04</b> Paper IV (Analytical Chemistry) <b>or</b>	3	--	--	3	80	20	40	100
	<b>01MSCCH05</b> Paper IV (Ind. Chem. & Env.) <b>or</b>	3	--	--	3	80	20	40	100
	<b>01MSCCH06</b> Paper IV (Green Chemistry) <b>or</b>	3	--	--	3	80	20	40	100
	<b>01MSCCH07</b> Paper IV (Hetcyc. & Nat. Prod.) <b>or</b>	3	--	--	3	80	20	40	100
	<b>01MSCCH08</b> Paper IV (Pharm. & Cosm. Chemistry)	3	--	--	3	80	20	40	100
<b>Practical</b>	<b>01MSCCHL1</b> Practical I (Based on Paper I & II)	--	--	4	2	75	25	50	100
	<b>01MSCCHL2</b> Practical II (Based on Paper III & IV)	--	--	4	2	75	25	50	100
<b>RM</b>	<b>01MSCCH09</b> Paper V (Research Methodology)	3			3	80	20	40	100
	<b>01MSCCHSI</b> Seminar I	1			1	-	50		50
	<b>Total</b>	<b>16</b>		<b>8</b>	<b>20</b>				<b>750</b>

<b>Scheme of Teaching and Examination for M.Sc. (Chemistry)</b>									
<b>M.Sc. (Chemistry) Semester – II</b>		<b>L</b>	<b>T</b>	<b>P</b>	<b>Total Credits</b>	<b>UA</b>	<b>CA</b>	<b>Min</b>	<b>Total</b>
<b>Major</b>	<b>02MSCCH01</b> Paper I (Inorganic Chemistry)	3	--	--	3	80	20	40	100
	<b>02MSCCH02</b> Paper II (Organic Chemistry)	3	--	--	3	80	20	40	100
	<b>02MSCCH03</b> Paper III (Physical Chemistry)	3	--	--	3	80	20	40	100
<b>Major Elective</b>	<b>02MSCCH04</b> Paper IV (Analytical Chemistry) <b>or</b>	3	--	--	3	80	20	40	100
	<b>02MSCCH05</b> Paper IV (Inorg. Mat. Of Ind. Imp.) <b>or</b>	3	--	--	3	80	20	40	100
	<b>02MSCCH06</b> Paper IV (Polymer Chemistry) <b>or</b>	3	--	--	3	80	20	40	100
	<b>02MSCCH07</b> Paper IV (Mol. Spectroscopy) <b>or</b>	3	--	--	3	80	20	40	100
	<b>02MSCCH08</b> Paper IV (Front. in Electrochemistry)	3	--	--	3	80	20	40	100
<b>Practical</b>	<b>02MSCCHL3</b> Practical III	--	--	4	2	75	25	50	100
	<b>02MSCCHL4</b> Practical IV	--	--	4	2	75	25	50	100
	<b>02MSCCH09</b> Paper V (OJT/FP)	3			3	80	20	40	100
	<b>02MSCCHS2</b> Seminar II	1			1	-	50		50
	<b>Total</b>	<b>16</b>		<b>8</b>	<b>20</b>				<b>750</b>

1. There will be five theory papers in every semester which will carry 80 marks each of 3 hrs. duration.
2. There will be internal assessment of 20 marks per paper per semester.
3. Each paper per semester with total of 100 marks (80 + 20) i.e. theory + internal assessment) will carry 3 credits.
4. The internal assessment will be based on Attendance, Home assignment, Unit test Terminal test and participation in departmental activities.
5. There will be two practical examinations in each semester i.e. Pract I and Pract II of 6-8 hours duration of 100 (75+ 25) marks with 2 credits each.
6. In each semester, the student will have to deliver a seminar on any topic relevant to the syllabus / subject encompassing the recent trends and development in that field / subject. This will carry 50 marks per seminar with one credit.
7. So, the total marks allotted to the Chemistry subject per semester is 750 marks: Theory (400 marks) + Internal assessment (100 marks) + Practicals (200 Marks) + Seminar (50 Marks) = 750 marks (total)
8. Each theory paper consists of four units of fifteen hours per unit. The following syllabi are prescribed on the basis of four hours per week of each paper and nine practical periods per batch per week.

<b>Scheme of Examination for M.Sc. (Chemistry)</b>			
<b>Semester I</b>	Internal Assessment	Theory Paper	Credits
<b>01MSCCH01</b> Paper I (Inorganic Chemistry)	20 Marks	80 Marks	3
<b>01MSCCH02</b> Paper II (Organic Chemistry)	20 Marks	80 Marks	3
<b>01MSCCH03</b> Paper III (Physical Chemistry)	20 Marks	80 Marks	3
<b>01MSCCH04</b> Paper IV (Analytical Chemistry) <b>or</b>	20 Marks	80 Marks	3
<b>01MSCCH05</b> Paper IV (Ind. Chem. & Env.) <b>or</b>	20 Marks	80 Marks	3
<b>01MSCCH06</b> Paper IV (Green Chemistry) <b>or</b>	20 Marks	80 Marks	3
<b>01MSCCH07</b> Paper IV (Hetcyc. & Nat. Prod.) <b>or</b>	20 Marks	80 Marks	3
<b>01MSCCH08</b> Paper IV (Pharm. & Cosm. Chemistry)	20 Marks	80 Marks	3
<b>01MSCCH09</b> Paper V (Research Methodology)	20 Marks	80 Marks	3
<b>01MSCCHL1</b> Practical I	25 Marks	75 Marks	2
<b>01MSCCHL2</b> Practical II	25 Marks	75 Marks	2
<b>01MSCCHSI</b> Seminar I		50 Marks	1
	<b>150 Marks</b>	<b>600 Marks</b>	<b>20</b>
<b>Semester II</b>	Internal Assessment	Theory Paper	Credits
<b>02MSCCH01</b> Paper I (Inorganic Chemistry)	20 Marks	80 Marks	3
<b>02MSCCH02</b> Paper II (Organic Chemistry)	20 Marks	80 Marks	3

<b>02MSCCH03</b> Paper III (Physical Chemistry)	20 Marks	80 Marks	3
<b>02MSCCH04</b> Paper IV (Analytical Chemistry) <b>or</b>	20 Marks	80 Marks	3
<b>02MSCCH05</b> Paper IV (Inorg. Mat. Of Ind. Imp.) <b>or</b>	20 Marks	80 Marks	3
<b>02MSCCH06</b> Paper IV (Polymer Chemistry) <b>or</b>	20 Marks	80 Marks	3
<b>02MSCCH07</b> Paper IV (Mol. Spectroscopy) <b>or</b>	20 Marks	80 Marks	3
<b>02MSCCH08</b> Paper IV (Front. in Electrochemistry)	20 Marks	80 Marks	3
<b>02MSCCH09</b> Paper V (OJT/FP)	20 Marks	80 Marks	3
<b>02MSCCHL3</b> Practical III	25 Marks	75 Marks	2
<b>02MSCCHL4</b> Practical IV	25 Marks	75 Marks	2
<b>02MSCCHS2</b> Seminar II		50 Marks	1
	<b>150 Marks</b>	<b>600 Marks</b>	<b>20</b>

### General scheme for distribution of marks in practical examination

Time : 6-8 h (One day Examination) Total Marks : 100 )

Internal 25

Exercise 75

Exercise-1 - 25 Marks

Exercise-2 - 25 Marks

Viva-Voce -15 Marks

Record -10 Marks

### Question Paper Pattern: Each paper comprising of Max marks 80 of 3 hours duration

Que.-1 (From Unit I) – (A-8 Marks + B-8 Marks) = 16 Marks or (a-4 + b-4 + c-4 + d-4 ) = 16 Marks

Que.-2 (From Unit II) – (A-8 Marks + B-8 Marks) = 16 Marks or (a-4 + b-4 + c-4 + d-4 ) = 16Marks

Que.-3 (From Unit III) – (A-8 Marks + B-8 Marks) = 16 Marks or (a-4 + b-4 + c-4 + d-4 ) = 16Marks

Que.-4 (From Unit IV) – (A-8 Marks + B-8 Marks ) = 16 Marks or (a-4 + b-4 + c-4 + d-4 ) = 16Marks

Que.-5 Short answer question each carry two marks (2 short questions from each unit)= 16 marks

Total: 80 marks

## Syllabus - NEP

### M.Sc. Semester – I

#### 01MSCCH01 Major DSC – Inorganic Chemistry – Paper - I

Credits : - Theory = 03      Practical = 02

Marks : - Theory = 100 (80 + 20)    Practical = 50

#### Unit – 1

##### A) Stereochemistry and Bonding in Main Group Compound: 5h

VSEPR-Shape of simple inorganic molecules and ions containing lone pairs, various stereo chemical rules and resultant geometry of the compounds of non-transitional elements, shortcomings of VSEPR model. Bent's rule and energetics of hybridization.

##### B) Metal – Ligand Bonding: 10h

Crystal Field Theory: Splitting of d-orbital in tetragonal, square planar and trigonal bipyramidal complexes. Jahn teller effect, spectrochemical series, nephelauxetic effect. Limitations of crystal field theory. M.O. theory for octahedral, tetrahedral & square planar complexes with and without  $\pi$ -bonding.

#### Unit – 2

##### A) Metal – Ligand Equilibria in Solution: 5h

Stepwise and overall formation constants; trends in stepwise formation constants; factors affecting stability of metal complexes with reference to nature of metal ion, ligand, chelate effect and thermodynamic origin. Determination of formation constant by : (1) spectrophotometric method (Job's and Mole ratio method) (2) Potentiometric method (Irving-Rossotti Method)

##### B) Reaction Mechanism of Transition metal complexes: 10h

Energy Profile of a reaction, reactivity of metal complexes, Inert and Labile complexes, Kinetics of Octahedral substitution: Acid hydrolysis, factors affecting acid hydrolysis, Stereochemistry of intermediates in  $SN_1$  &  $SN_2$  , Base hydrolysis, Conjugate base mechanism, Direct and indirect evidences in favour of conjugate mechanism, Anation reaction, reaction without metal-ligand bond breaking.

#### Unit 3 ~~Ionic Equilibria~~

##### Cluster- I 15h

Boron hydrides: Classification, nomenclature, structure, bonding and topology of borane 4-digit coding (s, t, y, x) numbers for higher boranes and their utilities. Chemistry of diboranes: Study of Metalloboranes, Carboranes and Metallocarboranes with reference to preparations and structures.

## Unit – IV A)

### Metal-Metal bonds: 10h

Occurrence of metal-metal bond, Classification of metal clusters, Binuclear, trinuclear, tetranuclear, pentanuclear and hexanuclear with reference to halide, oxide, alkoxide and acetate clusters.

B) Isopoly, Heteropoly acids and their anions. 5h

#### List of Books

- 1) S. F. A. Kettle, J. N. Murrell and S. T. Teddler: Valency Theory
- 2) C. A. Coulson: Valency
- 3) J. E. Huheey :Inorganic Chemistry
- 4) F .A. Cottonand G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5thand 6th Editions.
- 5) A. F. Williams: Theoretical Approach in inorganic chemistry.
- 6) A. Mannas Chanda: Atomic Structure and chemical Bonding
- 7) L. E. Orgel: An Introduction To transition metal chemistry, Ligand field theory, 2nd Ed.
- 8) J. J. Logowski: Modern Inorganic Chemistry
- 9) B.Durrant and P.J.Durrant: Advanced Inorganic Chemistry
- 10) J. C. Bailar: Chemistry of coordination compounds.
- 11) W. L. Jolly: Modern Inorganic Chemistry
- 12) R. S. Drago: Physical methods in inorganic chemistry.
- 13) Waddington: Nonaqueous solvents.
- 14) Sisler: Chemistry of nonaqueous solvents.
- 15) A. K. Barnard: Theoretical Inorganic Chemistry
- 16) Emeleus and Sharpe: Modern Aspect of Inorganic Chemistry.
- 17) F. A. Cotton: Chemical Applications of Group theory.
- 18) Jones: Elementary Coordination chemistry.
- 19) B. N. Figgis: Introduction to Ligand field.
- 20) S. F. A. Kettle: Coordination chemistry.
- 21) M.C.Day and J.Selbin: Theoretical Inorganic Chemistry.
- 22) J. Lewin and Wilkins: Modern Coordination Chemistry.
- 23) Gowarikar, Vishwanathan and Sheedar: Polymer science.
- 24) H. H. Jatney and M. Orchin: Symmetry in chemistry.
- 25) D. Schonaland: Molecular Symmetry in chemistry.
- 26) L. H. Hall: Group theory and Symmetry in chemistry
- 27) H. H. Jatney and M. Orchin: Symmetry in chemistry
- 28) R.L.Dutta and A.Symal: Elements of magneto chemistry
- 29) Inorganic Chemistry 4th Edition, P.Atkins, Oxford University Press.
- 30) Essential Trends in Inorganic Chemistry, D.M.P.Mingos, Oxford University Press.

## 01MSCCHL1- Laboratory – I

### Total Marks – 100 (75 + 25)

I. Preparation of Inorganic Complexes and their characterization by: Elemental analysis and physico-chemical methods (Electronic and IR Spectra, magnetic susceptibility measurements, Thermal analysis and Molar conductance studies).

1.  $K_3 [Al (C_2O_4)_3](H_2O)_3$

2.  $[\text{VO}(\text{acac})_2]$
3.  $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
4.  $\text{K}_3[\text{Cr}(\text{SCN})_6]$ .
5.  $[\text{Mn}(\text{acac})_3]$
6.  $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
7.  $\text{Hg}[\text{Co}(\text{SCN})_4]$
8.  $[\text{Co}(\text{Py})_2\text{Cl}_2]$
9.  $[\text{Cu}_2(\text{CH}_3\text{COO})_4(\text{H}_2\text{O})_2]$
10.  $[\text{Ni}(\text{DMG})_2]$
11.  $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
12.  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]\text{SO}_4$

### I. Qualitative analysis of radicals:

Semi-micro Analysis of inorganic mixture containing four cations out of which two will be rare metal ions such as W, Mo, Se, Ti, Zr, Ce, Th, V and U.

(Spot Test for individual cations should be performed)

### II. Quantitative Analysis:

Separation and determination of two metal ions from the following alloys involving: Volumetric, Gravimetric and Spectrophotometric methods.

- i) Copper (II) and Nickel(II)
- ii) Copper (II) and Zinc (II)
- iii) Nickel (II)—Zinc (II) and
- iv) Copper (II)—Iron (III)

## 01MSCCH02 Major DSC – Organic Chemistry, Paper - II

**Credits : - Theory = 03      Practical = 02**

**Marks : - Theory = 100 (80 + 20)    Practical = 100**

### Unit-I: 15 h

#### A] Nature and Bonding in Organic Molecule

Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyper-conjugation, bonding in fullerenes. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons Huckel's rule, energy level of  $\pi$  molecules orbitals, annulenes, antiaromaticity, homoaromaticity. Aromatic character and chemistry of cyclopentadienyl anion, tropylium cation, tropone and tropolone. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes

**B]** Synthetic applications of enamines and imines anions in organic synthesis, phase transfer catalysis, crown ethers and graphene.



## Unit-II: 15 h

### A] Stereochemistry

Conformational analysis of cycloalkanes (5 – 8 membered rings), substituted cyclohexanes, mono substituted, disubstituted and trisubstituted cyclohexanes, decalines, effect of conformation on reactivity, Cahn-Ingold-Prelog System to describe configuration at chiral centers. Elements of symmetry, chirality, molecules with more than one chiral center, meso compounds, threo and erythro isomers, method of resolution, optical purity, enantiotopic and distereotopic atoms, groups and faces, prochirality, addition-elimination reactions, stereospecific and stereoselective synthesis. Asymmetrical synthesis, optical activity in absence of chiral carbon (biphenyl and allenes)

### B] Reactive Intermediates

Generation, structure, stability and chemical reactions involving classical and non-classical carbocations, carbanions, free radical, carbenes, nitrenes and arynes. Singlet oxygen, its generation and reactions with organic substrates.

## Unit-III: 15 h

### A] Reaction mechanism:

Structure and Reactivity Types of mechanism, Types of reaction, thermodynamics and kinetics requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. Effect of Structure on reactivity: Resonance and field effects, Steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft Equation.

**B]** Concept of neighboring group participation (anchimeric assistance) with mechanism, neighboring group participation by  $\pi$  and  $\sigma$  bonds, classical and non classical carbocations, Intramolecular displacement by hydrogen, oxygen, nitrogen, sulphur and halogen. Alkyl, cycloalkyl, aryl participation, participation in bicyclic system, migratory aptitude, carbocation rearrangements and related rearrangements in neighboring group participation.

## Unit IV: 15h

**A] Aliphatic nucleophilic substitution** The  $S_N1$ ,  $S_N2$ , mixed  $S_N1$ ,  $S_N2$  and SET and  $S_Ni$  mechanisms. Nucleophilicity, effect of leaving group, ambient nucleophiles and ambient substrates regioselectivity, substitution at allylic and vinylic carbon atoms.

**B] Aromatic electrophilic substitution** The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The o/p ratio, ipsoattack, orientation in benzene ring with more than one substituents, orientation in other ring system. Diazonium coupling, Vilsmeier reaction, Gatterman-Koch reaction, Pechmann reaction, Reimer-Tiemann reaction, Diazonium coupling.

**C] Aromatic Nucleophilic Substitution** A general introduction to different mechanisms of aromatic nucleophilic substitution  $S_NAr$ ,  $S_N1$ , benzyne and  $S_{RN}1$  mechanisms. Reactivity - effect of substrate structure leaving group and attacking nucleophile. The Von Richter, Sommet-Hauser and Smiles rearrangements.

### List of books

- 1] Advanced Organic Chemistry –Reaction mechanism and structure. Jerry March, John Wiley
- 2] Advanced Organic Chemistry- F.A. Carey and R. J. Sunberg, Plenum
- 3] A Guidebook to Mechanism in Organic Chemistry-Peter Skyes, Longman
- 4] Structure and Mechanism in Organic Chemistry-C.K. Gold, Cornell University Press
- 5] Organic Chemistry, R.T. Morrison Boyd. Prentice Hall
- 6] Modern Organic Chemistry-H.O. House, Benjamin
- 7] Principal of Organic Chemistry-R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional
- 8] Reaction Mechanism in Organic Chemistry-S.M. Mukharji and S.P. Singh, Macmilan
- 9] Stereochemistry of Organic Compounds- D. Nasipuri, New Age International
- 10] Stereochemistry of Organic Compounds- P. S. Kalsi, New Age International
- 11] Frontier Orbitals and Organic Chemical Reactions-I. Fleming
- 12] Orbital Symmetry – R. E. Lehr and A. P. Marchand
- 13] Reactive Intermediate in Organic Chemistry-N. S. Isaacs
- 14] Stereochemistry of Carbon Compounds- E. L. Eliel
- 15] Physical Organic Chemistry-J. Hine
- 16] Name Reaction in Organic chemistry –Surrey
- 17] Advanced Organic Chemistry – L. F. Fieser and M. Fieser.
- 18] Organic Chemistry Vol. I and II - I. L. Finar
- 19] Modern Organic Chemistry- J.D. Roberts and M. C. Caserio
- 20] The Search for Organic Reaction Pathways (Longmann), Peter Skyes
- 21] Organic Chemistry 5th Edition (McGraw Hill), S. H. Pine
- 22] Organic Chemistry (Willard Grant Press Botcon), John McMurry
- 23] A Textbook of Organic Chemistry- R. K. Bansal New Age International
- 24] New Trends in Green Chemistry –V. K. Ahluwalia and M. Kidwai, Anamaya publishers
- 25] Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press
- 26] Organic Chemistry, 4th Edition, G Marc Loudon, Oxford University Press
- 27] Nano Materials 2007, A. K. Bandyopadhyay, New Age International.

## 01MSCCHL2 - Laboratory – II

**Total Marks – 100 (75+25)**

### 1] Qualitative Analysis

Separation, purification and identification of the mixture of two organic compounds (binary mixture with two solid, one solid one liquid and two liquids) using chemical methods or physical techniques. Minimum 8-10 mixtures to be analysed.

Purification of the compounds by crystallization, TLC and chromatographic techniques.

## 2] Organic preparations:

Student is expected to carry out minimum of 5-6 two stage organic preparation and 5-6 single stage preparation from the following lists.

- [1] Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.
- [2] Benzophenone → benzhydrol
- [3] Aldol condensation: Dibenzal acetone from benzaldehyde.
- [4] Sandmeyer reaction: p- chlorotoluene from p-toluidine
- [5] Cannizzaro reaction
- [6] Friedel Crafts Reaction:  $\beta$ -Benzoyl propionic acid from succinic anhydride and benzene.
- [7] Benzil \_ 2,4,5-triphenyl imidazole
- [8] Sucrose \_ Oxalic acid
- [9] Cyclohexanol\_ Adipic acid
- [10] Benzaldehyde \_ Dibenzal acetone
- [11] Phenol formaldehyde resin
- [12] Urea formaldehyde resin
- [13] Methyl acetoacetate \_ 5-methyl-isoxazol-3-ol
- [14] Ethyl acetoacetate → 4-aryl-6-methyl-3,4-dihydro-2(1H)-pyrimidinone ester
- [15] Ethyl acetoacetate → Diethyl 1,4-dihydro-2,6-dimethyl-4-phenylpyridine-3,-5dicarboxylate
- [16] Dye preparation : Sulphanilic acid → Methyl orange
- [17] Dye preparation : p-nitroaniline \_ p-red
- [18] Acetanilide → p-nitroacetanilide → p-nitroaniline
- [19] Aniline → 2,4,6-tribromo aniline → 2,4,6-tribromoacetanilide
- [20] Nitrobenzene → m-dinitrobenzene → m-nitroaniline
- [21] toluene → p-nitrotoluene → p-nitrobenzoic acid
- [22] Glycine → Benzoyl glycine → 4-benzilidene-2-phenyl oxazole
- [23] Phthalic anhydride → Phthalimide → Anthranilic acid [24] Resorcinol → fluorescein → Eosin

## 01MSCCH03 Major DSC – Physical Chemistry, Paper - III

**Credits : - Theory = 03      Practical = 00**

**Marks : - Theory = 100 (80 + 20) Practical = 100**

### UNIT I: FORMULATION OF QUANTUM MECHANICS 15h

**A]** Introduction of quantum mechanics, wave function, acceptability of wave functions, normalized and orthogonal wave functions, operators, properties of operators, eigen functions and eigen values, Hermitian operators, orbital and generalized angular momentum, eigen function and eigen values of angular momentum, postulates of quantum mechanics, (problems on operators, eigen values and average value)

**B]** Application of Schrodinger wave equation to simple systems: degeneracy in 3-dimensional box, rigid rotator, potential well of finite depth (tunneling effect), simple harmonic oscillator, the Hydrogen atom.

## **UNIT II: CLASSICAL THERMODYNAMICS 15h**

**A]** Exact and inexact differentials, condition of exactness, Pfaff differential expression, derivation of thermodynamic equation of state, extensive and intensive properties. Homogeneous functions of degree 0 and 1. Maxwell's relations.

**B]** Third law of thermodynamics, unattainability of absolute zero, calculation of entropy, residual entropy and its application. Varial equation, fugacity, determination of fugacity.

**C]** Partial molar quantities: Determination of partial molar quantities, chemical potential, escaping tendency, partial molar volume, Gibbs Duhem equation, Gibbs Duhem Mergules equation, reaction potential, Extent of reaction ( $\xi$ ).

## **UNIT III: PHASE EQUILIBRIA 15h**

Phase rule, calculation of degrees of freedom, reduced phase rule, construction of phase diagram, one component systems: Helium, carbon, two component systems forming solid solutions having congruent and incongruent melting point, partially miscible solid phase, three component systems, graphical presentation, influence of temperature, systems with 1, 2, 3 pairs of partially miscible liquids, transition points, 1st and 2nd order phase transition, lambda line.

## **UNIT IV: CHEMICAL KINETICS 15h**

**A]** Theories of reaction rates: Unimolecular reactions, bimolecular reactions, collision theory, steric factor, temperature effect on reaction rates, Arrhenius equation and its limitations, activation energy, transition state theory, steady state approximation, Lindeman-Hinshelwood mechanism, RRKM theory

**B]** Photochemistry: Introduction, quantum yield, photosensitizers, quenching, kinetics of anthrascene reactions,  $H_2-Br_2$  and  $H_2-I_2$  reactions.

**C]** Catalysis: Acid- base enzymes, enzyme catalysis, Michaelis Menten equation, effect of pH and temperature.

### **List of books**

1. Ira .N. Levine, Quantum Chemistry, 5th edition(2000), Pearson educ., Inc.New Delhi
2. A.K.Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata Mcgraw Hill, New Delhi.
3. S.K.Dogra, S.Dogra, Physical Chemistry Through Problems.
4. M.W.Hanna, " Quantum Mechanics in Chemistry", Benjamin
5. L. Pualing and E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York (1935).
6. R.P.Rastogi R.R. Mishra 6th revised edition An Introduction to Chemical Themodynamics.
7. Principles of Physical Chemistry by Puri, Sharma and Pathania,
8. P.W.Atkins.Physical chemistry. ELBS
9. E.N.Yenemin, " Fundamentals of Chemical Thermodynamics", MIR Publishers.

10. F.W.Sears, "Introduction to Thermodynamics, Kinetic Theory of Gases and statistical mechanics". Addison Wesley
11. G.M.Panchenkov and V.P.Labadev, "Chemical Kinetics and catalysis", MIR Publishing
12. E.A. Moelwyn- Hughes, "Chemical Kinetics and Kinetics of Solutions", Academic
13. K.J.Laidler, Chemical Kinetics, Third Edition (1987), Harper and Row, New York
14. J.Raja Ram and J.C.Kuriacose, Kinetics and Mechanism of Chemical Transformations MacMillan Indian Ltd., New Delhi (1993)
15. R.K.Prasad, "Quantum Chemistry", Wile

## **01MSCCH04 Major Elective I – Analytical Chemistry, Paper - IV**

**Credits : - Theory = 03**

**Marks : - Theory = 100 (80 + 20)**

### **Unit I: Introduction and statistical analysis 15h**

Introduction to analytical chemistry: Types of analysis-qualitative and quantitative. Classification of analytical methods- classical and instrumental, basis of their classification with examples. Statistical analysis and validation: Errors in chemical analysis. Classification of errors- systematic and random, additive and proportional, absolute and relative. Accuracy and precision. Mean, median, average deviation and standard deviation. Significant figures and rules to determine significant figures. Calculations involving significant figures. Confidence limit, correlation coefficient and regression analysis. Comparison of methods: F-test and T-test. Rejection of data based on Q-test. Least squares method for deriving calibration graph. Application of Microsoft Excel in statistical analysis (statistical functions and spreadsheets in MS-Excel). Validation of newly developed analytical method. Certified reference materials (CRMs). Numerical problems.

### **Unit II: Separation techniques 15h**

Chromatography: Definition and Classification. Techniques used in Paper, Thin Layer and Column chromatography. Applications in qualitative and quantitative analysis.

Ion exchange: Principle and technique. Types of ion exchangers. Ion exchange equilibria. Ion exchange capacity. Effect of complexing ions. Zeolites as ion-exchangers. Applications.

Solvent extraction: Principle and techniques. Distribution ratio and distribution coefficient. Factors affecting extraction efficiency: Ion association complexes, chelation, synergistic extraction, pH. Numericals based on multiple extractions. Role of chelating ligands, crown ethers, calixarenes and cryptands in solvent extraction.

Introduction to Solid phase extraction (SPE) and Microwave assisted extraction (MAE). Applications.

### **Unit III: Classical methods of analysis 15h**

Volumetric analysis: General principle. Criteria for reactions used in titrations. Primary standards and secondary standards. Theory of indicators. Types of titrations with examples- Acid-base, precipitation, redox and complexometric. Titration curves for monoprotic and polyprotic acids and bases. Indicators used in various types of titrations. Masking and demasking agents.

Gravimetric analysis: General principles and conditions of precipitation. Concepts of solubility, solubility product and precipitation equilibria. Steps involved in gravimetric analysis. Purity of precipitate: Co-precipitation and post-precipitation. Fractional precipitation. Precipitation from homogeneous solution. Particle size, crystal growth, colloidal state, aging and peptization phenomena. Ignition of precipitates.

## **Unit IV: Optical methods of analysis-I 15h**

Spectrophotometry and Colorimetry:

of colorimetry. Beer's law, its verification and deviations. Instrumentation in colorimetry and spectrophotometry (single and double beam). Sensitivity and analytical significance of molar extinction coefficient and  $\lambda_{\max}$ . Comparison method, calibration curve method and standard addition method for quantitative estimation. Role of organic ligands in spectrophotometric analysis of metal ions. Ringbom plot and Sandell's sensitivity. Photometric titrations. Determination of pK value of indicator. Simultaneous determination. Composition and stability constant of complex by Job's and mole ratio methods. Derivative spectrophotometry. Numerical problems.

### **List of books:**

1. Quantitative analysis: Day and Underwood (Prentice-Hall of India)
2. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3. Analytical Chemistry: Gary D. Christian (Wiley, India).
4. Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
5. Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
6. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
7. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
8. Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
9. Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
10. Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
11. An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
12. Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West
13. Instrumental Methods of Chemical Analysis: G. W. Ewing.

## 01MSCCH05 Major Elective II – Industrial Chemicals And Environment,

### Paper - IV

**Credits : - Theory = 03**

**Marks : - Theory = 100 (80 + 20)**

#### Unit- I

Industrial Gases and Inorganic Chemicals

**Industrial Gases:** Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.(2L)

**Inorganic Chemicals:** Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.(10 Lectures)

#### Unit II

**Industrial Metallurgy** Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology. (4 L)

Environment and its segments Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur. (2L)

Biocatalysis Introduction to biocatalysis: Importance in “Green Chemistry” and Chemical Industry. (6L)

#### Unit III

**Air Pollution:** Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; **Photochemical smog: its constituents and photochemistry.** Environmental effects of ozone, Major sources of air pollution. Pollution by SO<sub>2</sub>, CO<sub>2</sub>, CO, NO<sub>x</sub>, H<sub>2</sub>S and other foul smelling gases. Methods of estimation of CO, NO<sub>x</sub>, SO<sub>x</sub> and control procedures. Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates. (12 L)

#### Unit IV

**Energy & Environment** Sources of energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc.

Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management. (12L)

#### Reference Books

- 1 E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
- 2 R.M. Felder, R.W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
- 3 J. A. Kent: Riegel’s Handbook of Industrial Chemistry, CBS Publishers, New Delhi.

4 S. S. Dara: A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi.

5 K. De, Environmental Chemistry: New Age International Pvt., Ltd, New Delhi.

6 S. M. Khopkar, Environmental Pollution Analysis: Wiley Eastern Ltd, New Delhi

## **01MSCCH06 Major Elective III – Green Chemistry, Paper - IV**

**Credits : - Theory = 03**

**Marks : - Theory = 100 (80 + 20)**

### **UNIT I Introduction to Green Chemistry**

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Principles of Green Chemistry and Designing a Chemical synthesis. Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals – different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; (12 L)

**UNIT II** Examples of Green Synthesis/ Reactions, Green Synthesis of the following compounds: adipic acid, catechol, BHT, methylmethacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, disodium iminodiacetate (alternative to Strecker synthesis), citral, ibuprofen, paracetamol, furfural. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzoic acid), Oxidation (of toluene, alcohols).

Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Ortho ester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; (12L)

**UNIT III** Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizzaro reaction, Strecker synthesis, Reformatsky reaction. Selective methylation of active methylene group using dimethylcarbonate: Solid-state polymerization of amorphous polymers using diphenyl carbonate; Use of "Clayon", a non metallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses. (12L).

**UNIT IV** Future Trends in Green Chemistry, Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; on covalent derivatization; Green chemistry in sustainable



development,. Energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. (12 L).

## Reference Books

- 1 Anastas, P.T & Warner, J.C. Green Chemistry: Theory and Practice, Oxford University Press (1998).
- 2 Kirchoff, M. & Ryan, M.A. Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC (2002).
- 3 Ryan, M.A. Introduction to Green Chemistry, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
- 4 Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi. Bangalore C ISBN 978-93-81141-55-7 (2013).
- 5 Cann, M.C. & Connelly, M. E. Real world cases in Green Chemistry, American Chemical Society (2008).
- 6 Cann, M. C. & Thomas, P. Real world cases in Green Chemistry, American Chemical Society (2008).
- 7 Pavia, D. L. Lamponan, G. H. & Kriz, G.S. W B Introduction to organic laboratory.

## 01MSCCH07 Major Elective IV – Heterocycles and Natural Products, Paper - IV

**Credits : - Theory = 03**

**Marks : - Theory = 100 (80 + 20)**

### Unit - I

INTRODUCTION AND CHEMISTRY OF SMALL RING HETEROCYCLES  
Introduction, nomenclature, spectral characteristics, reactivity of heterocyclic compounds. Synthesis and reactions of three, four and five membered heterocycles (aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes, pyrrole, thiophene and furan).

### Unit - II

CHEMISTRY OF SIX MEMBERED AND BENZOFUSED HETEROCYCLES  
Synthesis and reactions of six membered heterocycles, pyridine, pyrylium salts, pyridinium & thiopyrylium salts. Chemistry of bicyclic compounds containing one or more heteroatom. Benzofused five and six membered rings: synthesis and reactions of

indoles, benzofuran, benzothiophene, quinolin, Isoquinoline, quinolones, isoquinolines, benzotriazoles, quinolinizium and benzopyrylium salts.

### **Unit – III**

#### **CHEMISTRY OF NATURAL PRODUCTS: TERPENOIDS, CAROTENOIDS AND STEROIDS**

Terpenoids and Carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Stereochemistry, Synthesis (chemical/biosynthesis) of the following representative molecules: Citral,  $\alpha$ -Terpeneol, Farnesol, Santonin, Phytol and  $\beta$ -carotene. Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation and biosynthesis of Cholesterol. Synthesis of Testosterone, Progesterone, Oestrone.

**Unit – IV** CHEMISTRY OF NATURAL PRODUCTS: ALKALOIDS AND FLAVONOIDS Alkaloids: Definition, nomenclature, occurrence, isolation, general methods of structure elucidation, classification based on nitrogen heterocyclic ring. Stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine, Atropine and Quinine. Flavonoids: Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids, Biosynthesis of flavonols and related polyphenols.

### **Reference Books:**

1. J. Clayden, B. Greeves and S. Warren, Organic Chemistry, Second Edition, Oxford University Press, 2012.
2. B. A. Bohm, Introduction to Flavonoids, Harwood Academic Publishers, 2011.
3. I. L. Finar, Organic Chemistry, Vol. 2, ELBS., 2009
4. Atta-ur-Rahman and Choudhary, Chemistry, Harwood Academic Publishers, 2008.
5. E. S. Coffey, Rodd's Chemistry of Carbon Compounds, Elsevier, 2005
6. J. A. Joule, Heterocyclic Chemistry, ELBS, 2005
7. Mann, Davidson, Hobbs, Banthrope and Harborne, Natural products: Chemistry and Biological Significance, Longman, Essex., 2004.
8. T. Eicher and S. Hauptmann, The Chemistry of Heterocycles, Thieme, 2002.
9. G. R. Newkome and W. W. Paudler, Contemporary Heterocyclic Chemistry, Wiley-Interscience, 1995.
10. T. L. Gilchrist, Heterocyclic Chemistry, Longman Scientific Technical, 1990.
11. R. M. Acheson, An Introduction to Heterocyclic Chemistry, John Wiley, 1980
12. A. R. Katritzky and C. W. Rees, Comprehensive Heterocyclic Chemistry, Pergamon Press, 1970.

1. K. L. Williamson and K. M., Masters Macroscale and Microscale Organic Experiments, 7th Edition. Cengage learning, 2017.
2. H.A. Shally, Green Chemistry Laboratory Manual for General Chemistry, CRC Press, 1st Edition, 2015.
3. D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, Introduction to Spectroscopy, 5th Edition. Cengage India, 2015.
4. R. M. Silverstein, G. C. Bassler and T. C. Morrill, Spectrometric Identification of Organic Compounds, 8th Edition, Wiley India, 2015.
5. William Kemp, Organic Spectroscopy, 3rd Edition. Mac publishers, 2011.
6. R. K. Bansal, Laboratory Manual in Organic Chemistry, Wiley, 2006.
7. Jag Mohan, Organic Spectroscopy, 2nd Edition. CRC Press, 2004.
8. B. S. Furniss and others, Vogel's Text Book of Practical Organic Chemistry, 5e Paperback, Pearson, 2003.
9. D. Pasto, C. Johnson and M. Miller, Experiments and Techniques in Organic Chemistry, Prentice Hall, Instructor's Edition, 1992.
10. H. T. Clarke revised by B. Haynee, A Hand book of Organic Analysis-Qualitative and Quantitative, Edward Arnold, London, 1975.
11. H. Middleton, Systematic Qualitative Organic Analysis, Edward Arnold, London, 1959.

## **01MSCCH08 Major Elective V – Pharmaceutical and Cosmetic Chemistry, Paper - IV**

**Credits : - Theory = 03**

**Marks : - Theory = 100 (80 + 20)**

**Unit – I** 1. Drugs & Pharmaceuticals: Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, Ibuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

**Unit – II** Fermentation Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

**Unit – III** Chemistry of Cosmetics & Perfumes: A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours.

**Unit – IV** Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

## Reference Books:

1. G.L. Patrick: Introduction to Medicinal Chemistry, Oxford University Press, UK.
2. Hakishan, V.K. Kapoor: Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan, Pitampura, New Delhi.
3. William O. Foye, Thomas L., Lemke , David A. William: Principles of Medicinal Chemistry, B.I. Waverly Pvt. Ltd. New Delhi.
4. E. Stocchi: Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK.
5. P.C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi. .
6. B.K. Sharma: Industrial Chemistry, Goel Publishing House, Meerut.

## 01MSCCH09 Minor – Research Methodology, Paper - V

**Credits : - Theory = 03      Seminar = 1**

**Marks : - Theory = 100      Seminar = 50**

### Unit – I METHODS AND TYPES OF RESEARCH

Research methods vs Methodology. Types of research, Descriptive vs. Analytical, Applied vs. Fundamental, Quantitative vs. Qualitative, Conceptual vs. Empirical. Research proposals- design and components.

### Unit – II LITERATURE REVIEW

Importance of literature review in defining a problem, Primary and secondary sources, reviews, treatise, monographs-patents, Defining and formulating the research problem, Selecting the Problems, Development of working hypothesis.

### Unit – III SCIENTIFIC SOFTWARES IN RESEARCH DESIGN

Data Analysis using Tools like MS Excel, ChemDraw and MATLAB, google scholar, chemspider, scifinder, scopus, reaxys, research gate; using advanced search techniques, web resources, e-journals, e-books, journal access, subscribing TOC alerts, hot articles, citation index, h-index and i-index, Impact factor.

### Unit – IV REPORTING, DOCUMENTATION AND PRESENTATION

Scientific Document; Organization and writing of research papers, short communications, review articles, monographs, peer reviewing, ethics in publishing, predatory journals and publishers, technical and survey reports, authored book and edited books and dissertation.

## References:

1. A. Fink, Conducting Research Literature Reviews: From the Internet to Paper, Sage Publications, 2009.

2. M. Graziano, A.M. Anthony and M. L. Raulin, Research Methods: A Process of Inquiry, Allyn and Bacon., 2009.
3. W. M. K. Trochim, Research Methods: the concise knowledge base, Atomic Dog Publishing, 2005.
4. P. D. Leedy and J. E. Ormrod, Practical Research: Planning and Design, Prentice Hall, 2004.
5. B. L. Garg, R. Karadia, F. Agarwal and U. K. Agarwal, An introduction to Research Methodology, RBSA Publishers, 2002.
6. R. A. Day, How to Write and Publish a Scientific Paper, Cambridge University Press, 1992.
7. C. R. Kothari, Research Methodology: Methods and Techniques, New Age International, 1990.
8. S. M. Coley and C. A. Scheinberg, Proposal Writing, Sage Publications, 1990.

### **01MSCCHS1 Seminar – I 50 marks**

Seminar of 30 minutes duration will be a part of internal assessment for 50 marks (1 credit). Seminar should be delivered by the student under the guidance of concerned teacher on the topic allotted by the teacher. The topic will be related to the syllabus. Marks will be allotted by a group of teachers.

## **Syllabus - NEP**

### **M.Sc. Semester – II**

#### **02MSCCH01 Major DSC – Inorganic Chemistry – Paper - VI**

**Credits : - Theory = 03**

**Marks : - Theory = 100 (80 + 20)**

#### **Unit I: A) Electronic spectra of Transition Metal complexes 10h**

Determining the Energy terms, Spin-orbit (L-S) coupling scheme, Hund's rule, Hole Formulation, Derivation of the term symbol for a d<sup>2</sup> configuration, Electronic spectra of transition metal complexes – Laporte 'orbital' selection rule, spin selection rule. Orgel diagrams for octahedral metal complexes. Charge transfer spectra, Racah parameters, calculations of  $10 Dq$ ,  $B$ ,  $\beta$  parameters. Tanabe-Sugano Diagrams of octahedral complexes with d<sup>2</sup> & d<sup>8</sup> configuration.

#### **B) Magnetic Properties of Transition Metal complexes 5h**

Abnormal magnetic properties, orbital contributions and quenching of orbital angular momentum, spin orbit coupling. Magnetic moment, electronic spectra and structure of tetrahalcobalt (II) complexes, tetrahedral and octahedral Ni(II) complexes. High spin-low spins crossover.

#### **Unit – II 15h**

##### **Reaction mechanism of Transition Metal Complexes-II**

Substitution reaction in square planer complexes: the trans effect, cis effect, steric effect, solvent effect, effect of leaving group, effect of charge, effect of nucleophile, effect of temperature. Trans effect theories, uses of trans-effect, mechanism of substitution reactions in Pt(II) complexes. Electron transfer reactions. Types of electron transfer reactions, conditions of electron transfer, and mechanism of one electron transfer reactions, outer sphere and inner sphere mechanisms, two electron transfer reactions complimentary and non-complimentary reactions. Tunneling effect, cross-reaction, Marcus-Hush theory, bridged activated mechanism.

#### **Unit-III: Metal pi-Complexes - I 15h**

##### **Metal carbonyls**

Structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls. Metal carbonyl clusters with reference to classification, EAN rule, synthesis and structures.

## Unit – IV: Metal $\pi$ -Complexes – II 15h

Metal nitrosyls Nitrosylating agents for synthesis of metal nitrosyls, vibrational spectra and X-ray diffraction studies of transition metal nitrosyls for bonding and structure elucidation, important reactions of transition metal nitrosyls, structure and bonding. Dinitrogen and dioxygen complexes. Wilkinson's catalyst and Vaska's compound.

### List of Books

1. J.E.Huheey :Inorganic Chemistry
2. F.A.Cotton and G. Wilkinson: Advanced Inorganic Chemistry 3rd, 5th and 6th Editions.
3. A.F. Willims: Theoretical Approach in inorganic chemistry.
4. Mannas Chanda: Atomic Structure and chemical Bonding
5. L. E. Orgel: An Introduction To transition metal chemistry, Ligand field theory, 2nd Edition.
6. J. J. Logowski: Modern Inorganic Chemistry
7. B.Durrant and P.J.Durrant: Advanced Inorganic Chemistry
8. J C. Bailar: Chemistry of coordination compounds.
9. W. L. Jolly: Modern Inorganic Chemistry Jones: Elementry Coordination chemistry.
10. B. N. Figgis: Introduction to Ligand field.
11. M.C.Day and J.Selbin: Therotical Inorganic Chemistry.
12. J. Lewin and Wilkins: Modern Co-ordination chemistry.
13. Purcell and Kotz: Inorganic Chemistry.
14. D. Banerjea: Co-ordination chemistry, Tata Mc. Graw. Pub.
15. A.F. Wells: Structural inorganic chemistry, 5th Edition, Oxford.
16. S. G. Davies: Organotransition metal chemistry applications to organic synthesis.
17. R. C. Mehrotra: Organometallic chemistry Tata McGraw Hill. Pub.
18. G. S. Manku: Thereotical priciples of inorganic chemistry
19. A. B. P. Lever: Inorganic electronic spectroscopy.
20. R.C.Maurya:Synthesis and charecterisation of novel nitrosyls compounds, Pioneer Pub. Jabalpur 2000.
21. R.H.Crabtree:The Organometallic chemistry of Transition metals, John Wiley.
22. D.N.Styanaryan:Electronic Absorption Spectroscopy and related techniques, University Press.
23. R. S. Drago: Physical methods in inorganic chemistry
24. F.Basolo and G.Pearson: Inorganic Reaction Mechanism
25. Organometallics II and I complexes with transition metal- carbon bonds: Manfred Bochmann-Oxford Press.
26. Advanced Inorganic Chemistry Vol I and II – Satyaprakash, Tuli, Bassu and Madan- S Chand.
27. M.Tsusui,M.Nlevy,M.Ichikwa and K.Mori:Introduction to metal  $\pi$ -complex chemistry,Plenum press,NY
28. A.E.Martel;Coordination Chemistry-VollandII,VNR.

## **02MSCCH02 Major DSC – Organic Chemistry – Paper - VII**

**Credits : - Theory = 03**

**Marks : - Theory = 100 (80 + 20)**

**Unit-I 15 h**

### **A] Addition to carbon-carbon multiple bond**

Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, Orientation and stereochemistry, Addition to cyclopropanes, Hydrogenation of double bond and triple bonds. Hydrogenation of aromatic rings, hydroboration, Michael reaction.

### **B] Addition to carbon-hetero atom multiple bond**

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters, and nitriles, Addition of Grignard reagents, organozinc and organolithium reagents to carbonyls and unsaturated carbonyl compounds, Wittig reaction, Mechanisms of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin, Stobbe reaction, Hydrolysis of esters and amide, ammonolysis of esters.

**Unit-II 15 h**

### **A] Mechanism of molecular rearrangement**

Classification and General mechanistic treatment of electrophilic, nucleophilic and free radical molecular rearrangement. Mechanism of the following rearrangement – Wagner-Meerwin, Pinacol-Pinacolone, Tiffenev –Demjnov ring expansion, benzil-benzilic acid, Arndt-Eistert synthesis, Curtius Lossen, Beckman, Hoffman, Schmidt rearrangement.

### **B] Free radical reactions-I**

Type of free radical reactions, free radical substitution mechanism at an aromatic substrate, aliphatic substrate, reactivity at a bridgehead position. Neighbouring group assistance, reactivity for aliphatic and aromatic substrates, reactivity in attacking radicals, effect of solvent on reactivity.

**UNIT-III**

### **A] Free radical reactions-II 15 h**

Halogenation at an alkyl carbon, allylic carbon (NBS), hydroxylation at an aromatic carbon by means of Fenton's reagent. Auto-oxidation, chlorosulphonation (Reed Reaction) Coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, Free radical rearrangement, Hunsdiecker reaction.

### **B] Elimination reactions**



The E1, E2 and E1CB mechanisms and orientation of the double bond. Saytzeff and Hoffman's rule. Effect of substrate structure, attacking base, leaving group and medium. Mechanism and orientation in pyrolytic elimination.

#### **Unit IV: Green chemistry 15 h**

Introduction, Education and need of Green chemistry, Basic principles of green chemistry. Prevention or minimization of hazardous products, choice of solvents. Sonochemistry, microwave induced reactions, polymer supported reagents, reactions in aqueous medium, zeolites and ionic liquid supported reaction, Solvent free reactions, Multi-component reactions (Biginelli, Ugi and Passereno reaction), Rearrangements reaction, Addition reaction, substitution, elimination reaction, photochemical and electrochemical reactions, Biocatalysts in Organic synthesis. Synthesis involving basic principles of green chemistry Synthesis of paracetamol and Ibuprofen, styrene, urethanes, Free radical bromination, Green chemistry for drug development, Synthesis of. Introduction to nanochemistry, nanorods and nanotubes.

#### **List of books**

- 1] Books as Suggested in Semester I for Organic Chemistry
- 2] A Textbook of organic chemistry- R.K. Bansal
- 3] New trends in green chemistry –V.K. Ahluwalia and M. Kidwai, Anamaya publishers New Delhi
- 4] Heterocyclic Chemistry, John Joule, Oxford University Press.

### **02MSCCH03 Major DSC – Physical Chemistry – Paper - VIII**

**Credits : - Theory = 03      Practical = 02**

**Marks : - Theory = 100 (80 + 20)    Practical = 100 (75 + 25)**

#### **UNIT I: APPLICATION OF QUANTUM MECHANICS 15h**

**A]** Approximate methods, variation principle, MO theory applied to H<sub>2</sub><sup>+</sup> molecule and H<sub>2</sub> molecule (calculation of energy), perturbation theory, application of perturbation theory to helium atom.

**B]** Electronic structure of atoms: Russel Sanders terms and coupling schemes, Slater-condon parameters, term separation energies of the pn configuration, term separation energies for dn configuraconfiguration, magnetic effects: spin orbit coupling and Zeeman splitting.

**C]** Hybridization, hybrid orbitals in terms of wave functions of s and p orbitals, sp and sp<sup>2</sup> hybridizations, Simple Huckel theory applied to: ethylene, butadiene, cyclobutadiene, cyclopropenyl radical.

#### **UNIT II: THERMODYNAMICS 15h**

**A]** Non-ideal Systems: Excess functions for non ideal solutions, Entropy of mixing, Enthalpy of mixing, Activity, activity coefficients, Debye Huckel theory for activity coefficients of electrolytic solutions, determination of activity and activity coefficients, ionic strength.

**B]** Statistical thermodynamics: Stirling Approximation, Maxwell Boltzmann, Bose Einstein, Fermi Dirac statistics, comparison between three statistics.

**C]** Irreversible Thermodynamics: Thermodynamic criteria for non equilibrium states, Le Chatelier principle, Conservation of mass and energy in closed and open systems, entropy production.

### **UNIT III: SOLID STATE CHEMISTRY 15h**

**A]** Crystal Defects and Non-stoichiometry: Perfect and imperfect crystals, Electronic structure of solids— band theory intrinsic and extrinsic defects- point defects, line and plane defects, vacancies- Schottky defects and Frenkel defects, p-n junction. Thermodynamics of Schottky and Frenkel defects, colour centres, non-stoichiometric defects. Superconductors—Meissner effect, BCS theory.

**B]** Solid State Reactions: General Principles, experimental procedures, co-precipitation as a precursor to solid state reactions, kinetics of solid state reactions.

### **UNIT IV: NUCLEAR CHEMISTRY 15h**

**A]** Introduction, radioactive decay and equilibrium, thermonuclear reactions, photonuclear reactions, Radiometric titration, isotopic dilution analysis, NAA.

**B]** Nuclear models: Fermi gas model, shell model, liquid drop model, application of liquid drop model semiempirical mass equation.

**C]** Counters: proportional counter, GM counter, scintillation counter, ionization chamber counter.

#### **List of books**

1. Ira N. Levine, Quantum Chemistry, 5th edition(2000), Pearson educ., Inc. New Delhi
2. A.K.Chandra, Introductory Quantum Chemistry, 4th edition (1994), Tata Mcgraw Hill, New Delhi.
3. S.K.Dogra, S.Dogra, Physical Chemistry Through Problems.
4. M.W.Hanna, " Quantum Mechanics in Chemistry", Benjamin
5. L. Pualing and E. B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York (1935).
6. R.P.Rastogi R.R. Mishra 6th revised edition An Introduction to CHEMICAL THERMODYNAMICS
7. Principles of Physical Chemistry by Puri, Sharma and Pathania, 8. Physical chemistry. P.W.Atkins.ELBS
9. E.N.Yenemin, "Fundamentals of Chemical Thermodynamics", MIR Publishers.
10. F.W.Sears, " Introduction to Thermodynamics, Kinetic Theory of Gases and statistical mechanics".Addison Wesley
11. M.C.Gupta, Statistical Mechanics
12. I.Prigogine, " An Introduction to Thermodynamics of Irreversible Processes," Interscience
13. Andrew Maczek, Statistical Thermodynamics, Oxford University Press Inc., New York (1998).

14. C.N.Rao. Nuclear Chemistry
15. B. G. Harvey, Introduction to Nuclear Physics and Chemistry, Prentice Hall, Inc. (1969).
16. H.J. Arnikar, Essentials of Nuclear Chemistry, 4th Edition (1995), Wiley-Eastern Ltd., New Delhi.
17. C.Kittel, " Introduction to solid state Physics", Wiley
18. L.V.Azaroff, " Introduction to solids", McGraw Hill.

## **02MSCCHL3 - Laboratory – III Practical – III**

**Total Marks – 100 (75 + 25)**

### **I**

1. To study the variation of volume contraction with mole fraction of alcohol in alcohol - water system
2. To determine the activation parameters of viscous flow for a given liquid
3. Determination of molecular mass of a polymer by viscometry method.
4. To determine integral heat of  $\text{KNO}_3$ , at two different conc. and calculation of heat of dilution.
5. Effect of 1% NaCl, 1% succinic acid, 0.5% naphthalene on CST in phenol-water systems.
6. Distribution of succinic acid in  $\text{H}_2\text{O}$ - benzene,  $\text{H}_2\text{O}$ -ether and comparison of distribution coefficient.
7. To construct the phase diagrams of two components system (phenol- urea, diphenyl aminebenzophenone; a-naphtyl amine-phenol) forming compounds with congruent melting points.
8. To study the mutual solubility of glycerol-m-toluidine and to determine congruent points.

### **II**

1. To study kinetics of hydrolysis of an ester by NaOH reaction.
2. To determine equilibrium constant of the equation  $\text{KI} + \text{I}_2 = \text{KI}_3$  by distribution method.
3. To study the kinetics of the reaction between potassium persulphate and potassium iodide.
4. Determination of order of reaction of oxidation of ethyl alcohol by acid dichromate.
5. To titrate conductometrically monobasic and dibasic acids with NaOH and determine the strength of given acid.
6. To determine equivalent conductance of weak electrolyte at infinite dilution by kaulrausch's method.
7. Determination of heat of reaction, entropy change and equilibrium constant of the reaction between metallic zinc and  $\text{Cu}^{+2}$  ions in solution.
8. Determination of thermodynamic constants  $\Delta G$ ,  $\Delta H$ ,  $\Delta S$  for  $\text{Zn} + \text{H}_2\text{SO}_4 = \text{ZnSO}_4 + 2\text{H}$  by emf measurement.

## **02MSCCH04 Major Elective I – Analytical Chemistry – Paper - IX**

**Credits : - Theory = 03      Practical = 02**

**Marks : - Theory = 100 (80 + 20)    Practical = 100 (75 + 25)**

### **Unit-I: Sampling and quantification 15h**

Sampling and sample treatment: Criteria for representative sample. Techniques of sampling of gases (ambient air and exhaust gases), liquids (water and milk samples), solids (soil and coal samples) and particulates. Hazards in sampling. Safety aspects in handling hazardous chemicals. Sample dissolution methods for elemental analysis: Dry and wet ashing, acid digestion, fusion processes and dissolution of organic samples.

Detection and quantification: Concepts and difference between sensitivity, limit of detection and limit of quantification, role of noise in determination of detection limit of analytical techniques. Units in chemical analysis and their interconversion. Stoichiometry: Stoichiometric and sub-stoichiometric reactions and calculations.

### **Unit- II: Modern separation techniques 15h**

Gas Chromatography: Principle including concept of theoretical plates and van-Deemter equation. Instrumental set up- carrier gas, sampling system, column and detector. Types of columns, their advantages and limitations. Detectors in GC analysis. Temperature programmed GC. Factors affecting retention, peak resolution and peak broadening.

Liquid chromatography: Principle, Instrumentation, Advantages and applications of HPLC. Types of columns and detectors. Principle and applications of size exclusion, gel permeation, ion retardation, normal phase and reverse phase chromatography. Supercritical fluid chromatography: Introduction and application.

### **Unit-III: Optical methods of analysis-II 15h**

Fluorometry and phosphorimetry: Principles of fluorescence and phosphorescence. Jablonski diagram. Concentration dependence of fluorescence intensity. Fluorescence quenching. Instrumentation. Applications.

Flame photometry: Principle. Instrumentation and types of burners. Factors affecting flame photometric determination. Limitations of flame photometry. Interferences in flame photometry. Applications. Nephelometry and turbidimetry: Theory, instrumentation and applications. Optical sensors: Fibre-optic properties, Fibre-optic sensors.

### **Unit-IV: Electrochemical methods of analysis-I 15h**

Polarography: Principle of DC polarography. Instrumentation in polarography. Advantages and limitations of DME. Types of currents- residual current, migration current, diffusion current, limiting current, adsorption current, kinetic current and catalytic current. Ilkovic equation-diffusion current constant and capillary

characteristics. Derivation of equation of polarographic wave and half wave potential. Experimental determination of half wave potential. Reversible, quasi reversible and irreversible electrode reactions. Polarographic maxima and maximum suppressor. Oxygen interference and deaeration. Introduction to pulse, a.c. and oscillographic techniques and their advantages. Applications of polarography in determination of dissolved oxygen, metal ion quantification and speciation, simultaneous determination of metal ions, analysis of organic compounds. Limitations of polarography. Amperometric titrations- Principle, types and applications in analytical Chemistry.

#### **List of books:**

1. Quantitative analysis: Day and Underwood (Prentice-Hall of India)
2. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3. Analytical Chemistry: Gary D. Christian (Wiley India).
4. Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
5. Sample Pre-treatment and Separation: R. Anderson (John Wiley and Sons)
6. Stoichiometry: B.I.Bhatt and S.M. Vora, 2nd Edition (Tata Mc-Graw Hill publication)
7. Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
8. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
9. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
10. Analytical Chemistry: Problems and Solution- S. M. Khopkar (New Age International Publication)
11. Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)
12. Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)
13. An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (WileyInterscience)
14. Fundamental of Analytical Chemistry: S. A. Skoog and D. W. West
15. Instrumental Methods of Chemical Analysis: G. W. Ewing
16. Polarography: Koltoff and Ligane
17. Electroanalytical Chemistry: Sane and Joshi (Quest Publications).

## **02MSCCHL4 Lab. – IV**

**Total Marks – 100 (75 + 100)**

### **(A): Classical methods and separation techniques**

Calibration, validation and computers

1. Calibration of pipette and burette.
2. Statistical analysis of data.
3. Use of MS-Excel in statistical analysis of data and curve fitting.

### **Volummetry**

1. Determination of  $\text{Na}_2\text{CO}_3$  in washing soda.
2. Determination of  $\text{NaOH}$  and  $\text{Na}_2\text{CO}_3$  in a mixture.
3. Estimation of nickel in given solution by direct complexometric titration with EDTA using bromopyrogallol red.

4. Estimation of nickel in given solution by complexometric back-titration with EDTA using murexide.
5. Estimation of chloride in given solution by Mohr's titration.
6. Estimation of chloride in given solution by Volhard's titration.
7. Determination of volume strength of commercial hydrogen peroxide by redox titration with  $\text{KMnO}_4$ .
8. Estimation of phenol/ aniline by bromination method.

### **Gravimetry**

1. Estimation of barium as barium sulphate.
2. Estimation of calcium as calcium oxalate/ calcium carbonate/ calcium oxide.

### **Separation techniques**

1. Qualitative separation of metal ions by paper chromatography for 2/3 components.
2. Determination of ion-exchange capacity of resin.

### **B] Instrumental techniques Electroanalytical techniques**

1. Analysis of commercial vinegar by conductometric titration.
2. Determination of strength of HCl and  $\text{CH}_3\text{COOH}$  in a mixture conductometrically.
3. Determination of strength of HCl and oxalic acid in a mixture conductometrically.
4. Determination of strength of oxalic acid and  $\text{CH}_3\text{COOH}$  in a mixture conductometrically.
5. Determination of degree of dissociation and dissociation constant of acetic acid conductometrically.
6. Determination of strength of HCl and  $\text{CH}_3\text{COOH}$  in a mixture potentiometrically.
7. Determination of Fe(II) by potentiometric titration with  $\text{K}_2\text{Cr}_2\text{O}_7$ .
8. Determination of three dissociation constants of  $\text{H}_3\text{PO}_4$  by pH-metric titration.

### **Optical methods**

1. Determination of pK of indicator by colorimetry.
2. To estimate the amount of  $\text{NH}_4\text{Cl}$  colorimetrically using Nessler's Reagent.
3. To study the complex formation between Fe(III) and salicylic acid and find the formula and stability constant of the complex colorimetrically (Job's method).
4. To determine the dissociation constant of phenolphthalein colorimetrically.

## **02MSCCH05 Major Elective II – Inorganic Materials of Industrial Importance – Paper - IX**

**Credits : - Theory = 03      Practical = 02**

**Marks : - Theory = 100 (80 + 20)    Practical = 100 (75 + 25)**

**UNIT I Silicate Industries & Glass:** Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre. Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements. (15 Lectures)

**UNIT II Fertilizers:** Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; mixed fertilizers, potassium chloride, potassium sulphate.

**Surface Coatings:** Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), (15 L)

**UNIT III Batteries:** Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solar cell and polymer cell.

**Alloys:** Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization and dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). (15 L).

## UNIT IV

**Catalysis:** General principles and properties of catalysts, Deactivation or regeneration of catalysts enzyme as nature's catalyst, Compare the activity and reactivity of man-made catalyst and enzyme, factors which affect enzyme activity,. Some industrially important catalytic process - Haber's, Ostwald's process, Phase transfer catalysts, application of zeolites as catalysts. (8 L)

Chemical explosives: Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants. (4 L).

## 02MSCCHL4 Lab. – IV

### Total Marks - 100 (75 + 100)

1. Determination of free acidity in ammonium sulphate fertilizer.
2. Estimation of Calcium in Calcium ammonium nitrate fertilizer.

3. Estimation of phosphoric acid in superphosphate fertilizer.
4. Electroless metallic coatings on ceramic and plastic material.
5. Determination of composition of dolomite (by complexometric titration).
6. Analysis of (Cu, Ni); (Cu, Zn ) in alloy or synthetic samples.
7. Analysis of Cement.
8. Preparation of pigment (zinc oxide).

### Reference Books

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: Introduction to Ceramics, Wiley Publishers, New Delhi.
4. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
5. P. C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
6. R. Gopalan, D. Venkappayya, S. Nagarajan: Engineering Chemistry, Vikas Publications, New Delhi.
7. B. K. Sharma: Engineering Chemistry, Goel Publishing House, Meerut.

## 02MSCCH06 Major Elective III – Polymer Chemistry – Paper - IX

**Credits : - Theory = 03      Practical = 02**

**Marks : - Theory = 100 (80 + 20)    Practical = 100 (75 + 100)**

**Unit I** Introduction and history of polymeric materials: Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers. Functionality and its importance: Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems. (15 L)

**Unit II** Kinetics of Polymerization: Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques. (8L) Polymer Additives Fillers & Reinforcement, Plasticizers, Antioxidants & Thermal Stabilizers (Heat Stabilizers), Ultraviolet stabilizers, Fire retardants, Colourants, Antistatic agents & Curing agents (7 L)

**UNIT III** Determination of molecular weight of polymers ( $M_n$ ,  $M_w$ , etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. (4 L)

Polymer Solution – Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of



mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.(8 L)

#### **UNIT IV**

Nature and structure of polymers-Structure Property relationships.(2 L)

Properties of Polymers (Physical, thermal, Flow & Mechanical Properties). Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylenesulphide)polypyrrole, polythiophene)].(10 L).

#### **02MSCCHL4 Lab. – IV**

##### **Total Marks – 100 (75 + 100)**

##### 1. Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA). a. Purification of monomer b. Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutyronitrile (AIBN)
2. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein a. Preparation of IPC b. Purification of IPC c. Interfacial polymerization
3. Redox polymerization of acrylamide
4. Precipitation polymerization of acrylonitrile
5. Preparations of novalac resin/resold resin.
6. Microscale Emulsion Polymerization of Poly (methylacrylate).

##### Polymer characterization

1. Determination of molecular weight by viscometry: (a) Polyacrylamide-aq.NaNO<sub>2</sub> solution (b) (Poly vinyl propylidene (PVP) in water
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
4. Testing of mechanical properties of polymers.

#### **Reference Books**

1. Seymour's Polymer Chemistry, Marcel Dekker, Inc.
2. G. Odian: Principles of Polymerization, John Wiley.
3. F.W. Billmeyer: Text Book of Polymer Science, John Wiley.

4. P. Ghosh: Polymer Science & Technology, Tata Mcgraw-Hill.
5. R.W. Lenz: Organic Chemistry of Synthetic High Polymers.

## **02MSCCH07 Major Elective IV – Molecular Spectroscopy – Paper - IX**

**Credits : - Theory = 03      Practical = 02**

**Marks : - Theory = 100 (80 + 20) Practical = 100**

**Unit – 1 ROTATIONAL SPECTROSCOPY** Basics of Molecular Spectroscopy  
Electromagnetic radiation and its region, representation of spectra, signal to noise ratio, resolving power, width and intensity of spectral lines. Rotational (Microwave) Spectroscopy Rotational Spectroscopy-Rigid diatomic Rotator, Selection rule for rotational/microwave spectrum, determination of bond-length, intensity of spectral lines, effects of isotopes on rotational spectra, Nonrigid rotator, Stark effect, Rotational spectra of linear polyatomic molecules, Application of microwave spectroscopy. 15

**Unit – II VIBRATIONAL AND RAMAN SPECTROSCOPY** Infrared (Vibrational) Spectroscopy Vibration in Diatomic molecules, Simple Harmonic Oscillator Model, Anharmonic Oscillator, Selection Rule, Population of Vibrational Energy level, Diatomic Vibrating Rotator, P-Q-R Branches of Spectra, Breakdown of Born Oppenheimer Approximation, Fundamental Vibration and their Symmetry, Overtone and Combination frequency, Applications of Infra-red spectroscopy. Raman Spectroscopy. Stokes and anti-Stokes lines. Polarizability ellipsoids. Pure Rotational Raman spectra, pure vibrational Raman spectra. Selection rules. Rule of Mutual Exclusion. Polarization of light, Raman Effect, Application of Raman and Infra-red spectroscopy in structure determination. (15)

**Unit – III ELECTRONIC SPECTROSCOPY** Principle of electronic spectroscopy, Total electronic angular momentum, Term symbol. Vibrational Coarse Structure: Progressions, Franck-Condon Principle, Dissociation energy and dissociation products, Rotational fine structure of electronic-vibration transitions, Fortrat diagram, Pre-dissociation.

**Unit – IV SOLID STATE AND SURFACE SPECTROSCOPY** Electronic Energy loss Spectroscopy (EELS), Reflection-Absorption Infrared Spectroscopy (RAIRS), Photoelectron spectroscopy (PES): X-ray PES and Ultra-violet PES, Auger Electron Spectroscopy (AES) and X-ray Fluorescence (XRF).

### **References:**

1. C. N. Banwell and E. M. Mc Cash, Fundamental of Molecular Spectroscopy, 4th Edition. Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2017.
2. D. N. Satyanarayana, Handbook of Molecular Spectroscopy: From radio waves to gamma rays, I. K. International Publishing House, New Delhi, 2015.
3. R. Kakkar, Atomic & Molecular Spectroscopy, Cambridge University Press, 2015.
4. J. M. Hollas, Modern Spectroscopy, 4th Edition. John Wiley & Sons, 2014.
5. G. E. Bacon, Fifty Years of Neutron Diffraction, Hilger, 2007.

6. B. E. Warren, X-Ray Diffraction, Dover Publications, 1999.
7. J. C. D. Brand and J. C. Speakman, Molecular Structure: The Physical Approach, 2nd Edition. Edward Arnold, London, 1995.
8. W. J. Moore, Physical Chemistry, 4th Edition. Prentice-Hall, 1992.
9. R. Chang, Basic Principles of Spectroscopy, McGraw-Hill, New York, 1990.

## **02MSCCHL4 Lab. – IV**

### **Total Marks – 100 (75 + 25)**

#### Spectrophotometry

1. Determine the concentration of Crystal violet and Aurine in mixture of (Crystal violet + Aurine) solution.
2. To determine the dissociation constant ( $K_a$ ) of Methyl red using UV-visible absorption spectrophotometer.
3. Verification of Beer law using solutions such as  $I_2$  in  $CCl_4$ , and  $CuSO_4$  in water,  $K_2Cr_2O_7$  and  $KMnO_4$  in sulphuric acid medium.

#### Potentiometry

1. To determine the strength of strong acid versus strong base, weak acid versus strong base, mixture of strong and weak acids versus strong base, weak acid versus weak base, strong acid versus weak base using a potentiometer.
2. To prepare and test the standard reference electrode i.e., calomel electrode or silver-silver chloride electrode.
3. Titrate Mohr's salt against  $KMnO_4$  potentiometrically and carry out the titration in reverse order.

#### Turbidimetry

1. To find the turbidity of given solution by using Nephthalo turbidity meter.
- #### Conductometry.
2. Study of conductometric titration of  $NH_4Cl$  versus  $NaOH$  solution,  $CH_3COONa$  versus  $HCl$ ,  $MgSO_4$  versus  $Ba(OH)_2$ ,  $BaCl_2$  and  $K_2SO_4$  and comment on the nature of graph.
  3. To study stepwise neutralization of polybasic acid like oxalic acid, citric acid, phosphoric acid by conductometric titration and explain the variation in the graph.

### **References:**

1. B. Viswanathan, P. S. Raghavan, Practical Physical Chemistry, M V Learning, 2017.
2. Shoemaker and Garland, Experiments in Physical Chemistry, McGraw Hill, 2015.
3. B. D. Khosla, V. C. Garg and Adarsh Gulati, Senior Practical Physical Chemistry, R. Chand & Co., New Delhi, 2014.
4. S. K. Maity and N. K. Ghosh, Physical Chemistry Practical, New Central book Agency, 2012.
5. G. P. Mathews, Experimental Physical Chemistry, 1st Edition. Oxford University Press, 1995.
6. A. M. James and F. E. Prichard, Practical Physical Chemistry, Lomgman, 1994.

7. B. P. Levitt, Findley's Practical Physical Chemistry, 9th Edition. Longman Group Ltd., 1993.
8. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 1991.
9. R. C. Das and B. Behara, Experimental Physical Chemistry, Tata McGraw Hill, 1984.

## **02MSCCH08 Major Elective V – Frontiers in Electrochemistry – Paper - IX**

**Credits : - Theory = 03      Practical = 02**

**Marks : - Theory = 100 (80 + 20)    Practical = 100 (75 + 25)**

**Unit – I ELECTRODICS** Rate of charge transfer reactions under zero field, under the influence of an electric field. The equilibrium exchange current density, the non-equilibrium drift-current density (Butler-Volmer) equation. High-field and low-field approximations. Physical meaning of the symmetry factor ( $\beta$ ), A simple picture of the symmetry factor and its dependence on over potential. Polarizable and nonpolarizable interfaces. (15)

**Unit – II FUEL CELLS, SUPERCAPACITORS AND BATTERIES** The maximum intrinsic efficiency, Actual efficiency and Current-Potential relation in an electrochemical energy converter. Factors influencing the electrochemical energy conversion, The power output of an electrochemical energy converter. Electrochemical electricity generators (fuel cells). Brief idea about H<sub>2</sub>-O<sub>2</sub> fuel cell, Hydrocarbon-air fuel cells, and Natural gas, CO-air fuel cells, Supercapacitors, and Lithium ion batteries. Electricity storage: Some important quantities in electricity storage (like electricity storage density, energy density and power), Desirable conditions for an ideal storer, Storage of electricity using the lead-acid battery, Dry cell, Silver-Zinc cell and Sodium-Sulfur cell. (15)

**Unit – III CORROSION** Electrochemistry of corrosion of metals, Factors affecting corrosion, Electrochemical cell formation, Polarization of metal electrode i.e. Concentration, Resistance and Activation polarization. Anodic and cathodic polarization curves (Evan's diagram). Electrochemical measurement of corrosion current density, corrosion potential and mixed potential theory and Tafel slope. Impedance spectroscopy technique, Anodic passivation and passivation potential. Passivity theory. Methods of protecting metal and their alloys from corrosion (anodic protection, cathodic protection, sacrificial protection, barrier protection, use of chemical inhibitors, environment modifiers).

### **References:**

1. M. G. Fontana, Corrosion Engineering, McGraw Hill, 2017.
2. H. K. Moudgil, Textbook of Physical Chemistry, PHI Publication House, New Delhi, 2015.
3. S. Glasstone, An introduction to Electrochemistry, Est West Press Ltd., 2016.

4. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry-I, Springer, 2009.
5. R. Narain, An Introduction to Metallic Corrosion, Oxford and IBH Pub Co., 1993.
6. P. Atkins and J. Paula, Atkins' Physical Chemistry, Oxford University Press, 10th ed., 2014.
7. D. Mcquarie and J. Simon, Physical Chemistry-A Molecular Approach, 1st Edition. Viva, 2010.
8. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry-I (Ionics), Springer, 2006.
9. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry-II, Springer, 2016.

## **02MSCCHL4 Lab. – IV**

**Total Marks – 100 (75 + 25)**

### **pH metric**

1. To determine the strength of strong acid versus strong base, weak acid versus strong base, mixture of strong and weak acids versus strong base, weak acid versus weak base, strong acid versus weak base using a pH meter.
2. To determine the concentration of a reductant or an oxidant i.e. Ferrous ammonium sulphate,  $K_2Cr_2O_7$  and  $KMnO_4$  by a pH metric titration method.
3. To determine the degree of hydrolysis and hydrolysis constant of aniline, acetic acid by pH metrically.

### **Conductometry**

1. Determination of the equivalent conductance of strong electrolytes such as HCl, KCl,  $KNO_3$ ,  $AgNO_3$  and NaCl and the validity of Onsager equation.
2. Determination of the solubility of lead sulfate and silver halides.
3. Conductometric titration of Strong acid vs. strong base, weak acid vs. strong base, Strong acid vs. weak base, weak acid vs. weak base using conductivity meter.

### **Polarimetry**

1. To determine the concentration of an optically active substance using polarimeter.
2. To determine the percentage of two optically active substances in a given mixture.

### **References:**

1. B. Viswanathan, P. S. Raghavan, Practical Physical Chemistry, M V Learning, 2017.
2. Shoemaker and Garland, Experiments in Physical Chemistry, McGraw Hill, 2015.
3. B. D. Khosla, V. C. Garg and Adarsh Gulati, Senior Practical Physical Chemistry, R. Chand & Co., New Delhi, 2014.
4. S. K. Maity and N. K. Ghosh, Physical Chemistry Practical, New Central book Agency, 2012.
5. G. P. Mathews, Experimental Physical Chemistry, 1st Edition. Oxford University Press, 1995.
6. A. M. James and F. E. Prichard, Practical Physical Chemistry, Longman, 1994.
7. B. P. Levitt, Findley's Practical Physical Chemistry, 9th Edition. Longman Group Ltd., 1993.

8. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 1991.
9. R. C. Das and B. Behara, Experimental Physical Chemistry, Tata McGraw Hill, 1984

### **02MSCCH09** Paper V (OJT/FP)

Student had to do On job training or Fellow project for 3 credits

### **02MSCCHS2 Seminar – II 50 marks Credit 01**

Seminar of 30 minutes duration will be a part of internal assessment for 50 marks (1 credit). Seminar should be delivered by the student under the guidance of concerned teacher on the topic allotted by the teacher. The topic will be related to the syllabus. Marks will be allotted by a group of teachers.



Chairman, BOS, Chemistry