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# **JAI PRAKASH UNIVERSITY CHAPRA**



**REGULATION AND COURSES OF STUDIES**

**FOR**

**Master of CHEMISTRY**

**BASED ON SEMESTER SYSTEM**

**w.e.f. The Session-2012-13**

**SYLLABUS**

M.Sc. Botany (Semester system)

w.e.f. 2012-2013

Jai Prakash University, Chapra



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**JAI PRAKASH UNIVERSITY, CHAPRA**



**BOARD OF COURSES OF STUDIES OF CHEMISTRY (P.G.)  
(FACULTY OF SCIENCES)**

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## COURSES OF STUDY FOR M .Sc. (CHEMISTRY)

The examination for M .Sc. (CHEMISTRY) course shall consist of four semesters having equally distribution of overall 80 credits with 1600 marks of sixteen papers. The duration of semester, distribution of credits and papers are as follows:

Name of Semester	Duration	Credits	* Papers
First Semester	July-December	20	4
Second Semester	January	20	4
Third Semester	July-December	20	4
Fourth Semester	January-June	20	4

The details of the course are as follows :

Semester Paper-Course-Code	Marks			Credits	Duration of Exam.	Teaching Hours
	U. Exam	Int. Eva.	Total			
1 <sup>st</sup> . 1-Phy.Che. [CH-101]	70	30	100	5	3h	90h
2-Inorg.Che. [CH-102]	70	30	100	5	3h	90h
3-Org.Che. [CH-103]	70	30	100	5	3h	90h
4-Phy.Che.Pr. [CH-104]	–	–	100	5	6h	270h
2 <sup>nd</sup> . 5-Quan.Che. [CH-201]	70	30	100	5	3h	90h
6-Coord.Che. [CH-202]	70	30	100	5	3h	90h
7-Che. Biom. [CH-203]	70	30	100	5	3h	90h
8-Inorg.Che.Pr. [CH-204]	–	–	100	5	6h	270h
3 <sup>rd</sup> . 9-Mol.Spect. [CH-301]	70	30	100	5	3h	90h
10-Biochem. [CH-302]	70	30	100	5	3h	90h
11-Envn-Anal. [CH-303]	70	30	100	5	3h	90h
12-Org.Che.Pr. [CH-304]	–	–	100	5	6h	270h

Each student has to opt only one elective subject as specialization from the list of the groups of subjects offered in the 4th semester.

Semester	Paper-Course-Code	Marks			Credit	Duration of Exam.	Teaching Marks
		U. Exam	Int. Eva.	Total			
<b>4<sup>th</sup>. Group-A [Physical Chemistry Specialization]</b>							
	13-Adv.Quan.Che. [Ch-401-P]	70	30	100	5	3h	90
	14-Mol.Therm. [CH-402-P]	70	30	100	5	3h	90h
	15-Che.Dynamics [CH-403-P]	70	30	100	5	3h	90h
	16-Phy.Che.Pr.Spl. [CH-404-P]	–	–	100	5	12h	270h
<b>Group-B [Inorganic Chemistry Specialization]</b>							
	13-Ligand Field Theory [Ch-401-I]	70	30	100	5	3h	90h
	14-Reac.Mech.Supramol. [CH-402-I]	70	30	100	5	3h	90h
	15-Org.Trans.Metal Che. [CH-403-I]	70	30	100	5	3h	90h
	16-Inorg.Che.Pr.Spl. [CH-404-I]	–	–	100	5	6h	270h
<b>Group-C [Organic Chemistry Specialization]</b>							
	13-Org.Synthesis [Ch-401-O]	70	30	100	5	3h	90h
	14-Natural Products [CH-402-O]	70	30	100	5	3h	90h
	15-Med. & Heterocycl. [CH-403-O]	70	30	100	5	3h	90h
	16-Org.Che.Pr.Spl. [CH-404-O]	–	–	100	5	6h	270h

The theory question paper of every end semester may comprise of long, short and objective type questions covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows :

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees. The detailed syllabi will be as follows :

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## 1<sup>st</sup> SEMESTER

**PAPER-1**

**PHYSICAL CHEMISTRY [CH-101]**

**Marks-70**

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees. The detailed syllabi will be as follows :

### Unit -1: CHEMISCAL THERMODYNAMICS

(a) Partial molar properties: Free energy, Entropy, Enthalpy, Volume, etc. in ideal gas mixture; variation of chemical potential with temperature and pressure, Determination of Chemical Potential, Gibbs-Duhem Equation.

Fugacity and Activity, their variation with T and P, Fugacity of a gas mixture, Lewis-Randall rule & its significance.

(b) Thermodynamics of ideal and non-ideal solution. Duhem-Margules equation and its application.

(c) Ensembles, Thermodynamic Probability, Boltzmann-Planck Equation, Concept of energy distribution-Boltzmann distribution law. Partition function and its significance, Relationship between Thermodynamic function and Partition function, Sackur-Tetrode Equation.

### Unit-2: CHEMICAL KINETICS

(a) Mechanism and kinetics of consecutive, opposing and side reactions.

(b) Evaluation of activation parameters ( $AE^*$ ,  $AH^*$ ,  $AG^*$ ,  $AS^*$ , etc), ARRT and rate of reaction in bi and tri-molecular gas phase reactions, reaction coordinate and potential energy surfaces for simple reactions.

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- (b) Evaluation of activation parameters ( $AE^*$ ,  $AH^*$ ,  $AG^*$ ,  $AS^*$ , etc), ARRT and rate of reaction in bi and tri-molecular gas phase reactions, reaction coordinate and potential energy surfaces for simple reactions.
- (c) Mechanism and Kinetics of Photolysis of acetaldehyde, and Photo-dimerisation of Anthracene-Quenching of Fluorescence, Stern-Volmer Equation.

### **Unit-3 : ELECTRO CHEMISTRY**

- (a) Electrode potential in terms of chemical potential and activity, Thermodynamics of cell reaction.
- (b) Debye Huckel - Onsager treatment and its extension, ion-solvent interactions, Debye Huckel -Jerum mode.
- (c) Over potential, exchange current density, Derivation of Butler-Volmer equation, Tafel Plot.
- (d) Polarography theory, Ilkovic equation, half wave potential and its significance.

### **Unit-4 : CHEMICAL CRYSTALLOGRAPHY & BAND THEORY**

Crystal symmetry, space groups, interplanar spacing, indexing of planes, Powder pattern, Determination of lattice type and unit cell dimensions of NaCl and KCl crystals, structure factor and crystal analysis of cubic system, electron density distribution.

Band theory of metals, insulators and semiconductors, types of semi-conductors, doping semiconductors, p-n junctions, super conductors, optical reflectance, photoelectric effect, classification of materials based on magnetic properties, hysteresis, Organic solids or metals.

### **Unit-5 : INTERFACE CHEMISTRY**

Surface free energy, surface films on liquids, vapour pressure of droplets, Gibbs Adsorption isotherm, BET Theory.

#### **Books Recommended :**

1. Modern Electrochemistry, Vol. 2 A & B, J.O'M. Bockris and A. K. N. Reddy, 2nd Ed. Plenum Press, New York (1998).
2. Chemical Kinetics, K. J. Laidler, 3rd Ed. (1987), Harper & Row, New York.
3. Physical Chemistry, P. W. Atkins, 8th Edn. Oxford University Press, New York.
4. Physical Chemistry, I.N. Levine, 5th Edn. Tata McGraw Hill Pub. Co. Ltd., New Delhi.

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees. The detailed syllabi will be as follows :

#### Unit-1 : STEREOCHEMISTRY AND BONDING OF COMPOUNDS OF MAIN GROUP.

VSEPR theory, d<sup>2</sup>-p<sup>2</sup> bond, Bent rule, M.O. diagram for CO<sub>2</sub>, NO<sub>2</sub><sup>-</sup>, CO<sub>3</sub><sup>2-</sup> and Xenon fluorides, electron deficiency and structural aspects of boranes, carboranes. Wade's rule, Metal-Metal multiple bonding, Fluxional compounds

#### Unit-2 : NUCLEAR CHEMISTRY

Shell Model liquid drop model, nuclear reactions and their types, nuclear reaction cross section. Detection and measurement of radiation G.M. and Scintillation counters, Nuclear reactors Application of radio isotopes, tracer technique, neutron activation analysis, isotopic dilution method, radiation hazards

#### Unit-3 : CHEMISTRY OF F-BLOCK ELEMENTS

Shape & orientation of f-orbitals, position in periodic table, separation technique: Ion exchange and solvent extraction methods, Lanthanide and actinide contractions, Magnetic and spectral properties, transuranic elements, synthesis and chemistry of Np and Pu, Separation of Pu from Spent fuel.

#### Unit-4 : SYMMETRY OPERATION AND ASSOCIATED SYMMETRY ELEMENTS

Classification of molecules into point groups, Defining properties of a mathematical group, Symmetry operation of a molecules as elements of a mathematical group, subgroups, concept of conjugate and class, multiple operations and group multiplication table in simple cases-C<sub>2v</sub>, C<sub>2h</sub> and C<sub>3v</sub>.



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## Unit-5 : MATRIX REPRESENTATIONS FOR SYMMETRY OPERATIONS

Reducible and Irreducible representations, Characters, the great orthogonality theorem (derivation not required), Consequences of orthogonality theorem, character table, construction of character table for  $C_{2v}$ ,  $C_{2h}$  and  $C_{3v}$  direct product, reduction formula, transformation of A.Os. under different point groups.

### Books Recommended :

1. *Advanced Inorganic Chemistry*, F.A. Cotton and G. Wilkinson, 6th Edn. (1999), John Wiley & Sons, New York.
2. *Inorganic Chemistry*, James E. Huheey, 4th Edn. (1993), Addison-Wesley Pub. Co., New York.
3. *Physical Methods in Inorganic Chemistry*, R. S. Drago, International Edn. (1971), Affiliated East-West Press, New Delhi.
4. *Inorganic Chemistry*, Keith F. Purcell and John C. Kotz, W. B. Saunders Com. (1987), Hong Kong.
5. *Symmetry and Spectroscopy of Molecules*, K. Veera Reddy, New Age International Pvt. Ltd., New Delhi (1999).

## PAPER-3

## ORGANIC CHEMISTRY [CH-103]

Marks-70

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees. The detailed syllabi will be as follows :

### Unit-1 : STEREOCHEMISTRY

Conformational analysis of cycloalkanes, Decalins, Steric strain due to unavoidable crowding, chirality, molecules with more than one chiral centre, methods of resolution, optical activity in the absence of chiral carbon (biphenyl's, allenes and spiranes), chirality due to helical shape, stereo-

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chemistry of the compounds containing nitrogen, sulfur and phosphorus, elementary idea of optical rotator dispersion and circular dichorism.

### **Unit-2 : REACTION MECHANISM: STRUCTURE AND REACTIVITY**

Types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammonds's postulate, Curtin-Hammett principle, potential energy diagram, Transition states and intermediates, Methods of determining mechanism, isotope effect, Hard and Soft acids and bases, Generation, Structure, Stability and reactivity of carbocations, carbanions, Free radicals, carbenes and nitrenes, effect of structure on reactivity, resonance and field effects, steric effect, the Hammett equation and Linear free energy relationship, substituent and reaction constants.

### **Unit-3 : AROMATIC SUBSTITUTION**

Aromaticity in benzenoid and non-benzenoid compounds, Huckel's rule, Energy level of molecular orbital's, Annulenes, Anti-aromaticity, PMO approach, S<sub>N</sub>Ar : S<sub>N</sub>1Ar, S<sub>N</sub>2Ar, Benzyne mechanism, effects of substrate structure, leaving group and attacking nucleophile on reactivity, Von Richter, Sommelet-Hauser and Smiles rearrangement.

### **Unit-4 : FREE RADICAL REACTIONS**

Free radical substitution mechanism, mechanism at on aromatic substrate, reactivity for aliphatic and aromatic substrates at bridgehead, The effect of solvent on reactivity, allylic halogenations, coupling of alkynes, arylation of aromatic compounds and active alkenes by diazonium salts, Sandmeyer reaction, Hunsdiecker reaction.

### **UNIT-5 : ADDITION TO MULTIPLE BONDS**

- (a) Mechanism and stereochemical aspects of addition reactions involving electrophile, nucleophile and free radicals, regioselectivity, orientation and reactivity, Hydroboration, Michael Addition
- (b) Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids and esters, Stobbe reaction.

### **UNIT-6 : ELIMINATION REACTIONS**

The E1, E2 and E1cB mechanisms, orientation of the double bond, reactivity-effects of substrate structure, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

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**Books Recommended:**

1. *March's Advanced Organic Chemistry*, M. B. Smith & Jerry March, 5th Edition (2001), John Wiley & Sons, New York.
2. *A Guide book to Mechanism in Organic Chemistry*, Peter Sykes, 6th Edition (1997), Orient Longman Ltd., New Delhi.
3. *Reaction Mechanism in Organic Chemistry*, S. M. Mukherjee and S. P. Singh, 1st Edition (1990), Macmillan India Ltd., New Delhi.
4. *Mechanism and Theory in Organic Chemistry*, T. H. Lowry and K. S. Richardson, 3rd Edn. Addison - Wesley Longman Inc. NY.
5. *Organic Reactions and their Mechanisms P.S. Kalsi*, 1st Edition (1996), New Age International Publication, New Delhi.

**PAPER-3 PHYSICAL CHEMISTRY LAB COURSE [CH-104] Marks-100**

The paper consists of following units:

**Unit-1: EXPERIMENTS**

One experiment is to be carried out among following list of experiments : 70 × 1marks

- Water equivalent of calorimeter and determination of
  - Heat of solution of potassium nitrate.
  - Heat of neutralization of strong acid and strong base.
  - Basicity of polybasic acids.
2. Determination of rate constant of hydrolysis of methyl acetate in acid medium.
  3. To study saponification of ethyl acetate by sodium hydroxide and determination of rate constant.
  4. To determine the distribution coefficient of  
(i) Acetic acid and (ii) benzoic acid
  5. Determination of specific and molecular and molecular rotation of sucrose in different concentrations and to determine the concentration of given solution.
  6. Determination of rate constant for inversion of cane sugar polarimetrically.
  7. Conductometric determination of:
    - Dissociation of constant of acetic acid.
    - Acid-base titration of NaOH and HCl solutions.

- ⇒ Mixture of HCl and CH<sub>3</sub>COOH with NaOH.
  - ⇒ Solubility product of sparingly soluble salt.
- Potentiometer determination of :
- (i) EMF of concentration cell.
  - (ii) pH of a given solution using SHE and quinhydrone electrode.

**Unit-2: Record** 05

**Unit-3: Viva-voce** 25

**Books Recommended :**

1. *Experiments in Physical Chemistry*, R. C. Das and B. Behra, Tata McGraw Hill.
2. *Advanced Practical Physical Chemistry*, J. B. Yadav, Goel Publishing House.
3. *Advanced Experimental Chemistry*, Vol-I-Physical. J. N. Gurtu and R. Kapoor, S. Chand & Co.
4. *Selected Experiments in Physical Chemistry*, N. C. Mukherjee, J. N. Ghose & Sons.
5. *Experiments in Physical Chemistry*, J. C. Ghose, Bharati Bhawan.

## 2<sup>nd</sup> SEMESTER

**PAPER-5**

**QUANTUM CHEMISTRY [CH-201]**

**Marks-70**

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Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The detailed syllabi will be as follows :

The paper consists of following units :

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## Unit-1 : INTRODUCTION TO QUANTUM MECHANICS

Basic postulates, quantum mechanics operators such as Hamiltonian and angular momentum operators, theorems, Schrodinger wave equation in operator form, Eigen function and Eigen value, Linear and Hermitian operators, commutation relationship.

## Unit-2 : EXACTLY SOLUBLE SYSTEMS IN QUANTUM MECHANICS

### H-Like Atom :

Separation of  $r$ ,  $\theta$  and  $\phi$  equation and procedure of solving them such as Laguerre differential equation and Legendre differential equation, concept of atomic orbital's, most probable distance and average distance in case of H-atom in ground state.

### Linear Harmonic Oscillator :

Harmonic Vibrations, solution of linear H.P. through Hermite differential equation using recursion formula, zero point energy, Eigen functions and Eigen values for vibrational level,

## Unit-3 : APPROXIMATION METHODS

Variation method-nonlinear and linear, application to harmonic oscillator and He atom, perturbation method-First order perturbation application to He atom, Secular equation, Slater determinant, singlet and triplet states in He atom, energy of ground state and excited state of He atom, symmetric and antisymmetric wave functions, coulomb and exchange integrals, antisymmetry rules and Pauli principle.

## Unit-4 : VALENCE BOND AND MOLECULAR ORBITAL THEORY

Principles of superposition, V.B. treatment of  $H_2$  molecule, V.B. wave functions, resonance integral, coulomb integral, overlap integral, charge density, LCAO approximation, M.O. treatment of  $H_2^+$  and  $H_2$ , representations for and molecular orbital's, comparison between V.B. and M.O. theories.

## Unit-5 : HUCKEL MOLECULAR ORBITAL THEORY

HMO theories for conjugated systems, calculation of bond order, free valence & charge density for ethylene, allyl skeleton and butadiene using HMO approximations.

### Books Recommended :

1. *Quantum Chemistry*, I.N. Levine, 5th Edition (2000), Pearson Educ., Inc. New Delhi.
2. *Physical Chemistry: A Molecular Approach*, D.A. Mc Quarrie & J.D. Simon, (1998) Viva Books, New Delhi.
3. *Valence Theory*, J. N. Murrell, S. F. A. Kettle & J. M. Tedder, 2nd Edition (1965), John Wiley, New York.
4. *Introductory Quantum Chemistry*, A.K. Chandra, 4th Edition (1994), Tata Mc-Graw Hill, New Delhi.
5. *Quantum Chemistry*, R.K. Prasad, New Age International, New Delhi.

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Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees. The detailed syllabi will be as follows :

The paper consists of following units :

#### UNIT-1 : BONDING IN COORDINATION COMPOUNDS

Crystal field theory, d-orbital splitting in cubic and non cubic fields, Measurement of  $10 Dq$  and its affecting factors, splitting of S, P, D and F terms in Octahedral and Tetrahedral symmetry, Limitations of C.F.T.

Evidences in support of covalent bonding in transition metal complexes, M.O. theory for  $ML_6$  with ? and ? bonding ligands using symmetry arguments, magnetic properties and charge transfer spectra on the basis of M.O. model.

#### UNIT-2 : MAGNETIC NATURE OF SUBSTANCES

The orbital and spin effects of paramagnetism, derivation of Russel- Sounder's terms, spin-orbit interaction, magnetic moment for large and small multiplet width, Quenching of orbital contribution, magnetic properties of complexes.

#### UNIT-3 : SPECTRAL AND THERMODYNAMIC ASPECTS OF C. F.T.

Electronic Spectra: selection rules for d-d transitions, and its breakdown, Electronic spectra of  $d_1$ ,  $d_2$ ,  $d_3$  and  $d_4$  systems, spectro-chemical series, crystal field effect on ionic radii of 3d ions, Jahn-Teller distortion, thermodynamic effects, lattice energy and hydration energy of octahedral complexes of 3d series, Site selection in normal and inverse spinel structures.

Step wise and overall stability constants, determination of stability constant by Bjerrum and e.m.f. methods, Job's continuous variation method.

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#### UNIT-4 : SUBSTITUTION REACTION IN TRANSITION METAL COMPLEXES

Nature of substitution reaction, liability and inertness of complexes, dissociative and associative mechanisms, substitution reaction in octahedral Co (III) complexes, acid and base hydrolysis, SN1CB hydrolysis, factors governing the rate of reaction, substitution without cleavage metal-ligand bond.

#### UNIT-5 : COMPLEXES WITH ACID LIGANDS

Synthesis, structure, bonding and reactions of nitrosyls and tertiary phosphine metal complexes.

#### Books Recommended :

1. *Structural Methods in Inorganic Chemistry*, E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.
2. *Inorganic Chemistry*, G. L. Miessler and D. A. Tarr, 2nd Edn. (1999), Prentice Hall International Inc., London.
3. *The Organometallic Chemistry of Transition Metals*, R. H. Crabtree, John Wiley.
4. *Inorganic Reaction Mechanisms*, Martin L. Tobe and John Burgess, Longmans 1st Edn. (1999).  
*Mechanism of Inorganic Reactions*, F. Basco and R. G. Pearson, 2nd Edn (1967), Wiley Eastern Ltd., New Delhi.
5. *Inorganic Chemistry*, D. F. Shriver and P. W. Atkins, 3rd Edn. (1999), ELBS, London.
6. *Introduction to Ligand Fields*, B.N. Figgis, Wiley Eastern Ltd. New Delhi (1976).

#### PAPER-7 CHEMISTRY OF BIOMOLECULES [CH-203] Marks-70

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The paper consists of following units :

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## UNIT - 1 : CARBOHYDRATES

Disaccharides - structure determination and chemical synthesis (Sucrose, Lactose & Maltose).

Polysaccharides - structure of Cellulose, Starch and Glycogen.

## UNIT- 2 : AMONO ACIDS AND PROTEINS

Amino acids – essential, non-essential, isoelectric point, primary structure of proteins, secondary structure of proteins, forces responsible for secondary structure of proteins,  $\alpha$ -helix &  $\beta$ -sheet structures of proteins, tertiary & quaternary structures of proteins.

## UNIT - 3 : NUCLEOTIDES AND NUCLEIC ACIDS

Chemical syntheses of purine and pyrimidine bases present in nucleic acids, structures of nucleosides and nucleotides, structures of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helical model of DNA.

## UNIT- 4 : TERPENOIDS

Introduction, classification, isoprene rule, structure determination and synthesis of terpineol, citral & camphor.

## UNIT - 5 : ALKALOIDS

Introduction, classification, structure determination and synthesis of nicotine and papaverine.

### Books Recommended :

1. *Lehninger Principles of Biochemistry*, D.L. Nelson and M.M. Cox, 3rd Edition ((2002) McMillan North Publication.
2. *Chemistry of the Alkaloids*, S.W. Pelletier, Van Nostrand Reinhold Co., New York (1970).
3. *Organic Chemistry*, I. L. Finar, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi.
4. *Total Synthesis of Natural Products*, J.W. Apsimon, Vol. 1-6, Wiley-Interscience Publications, New York.
5. *Creativity in Organic Synthesis*, J.S. Bindra and R. Bindra.
6. *Organic Chemistry*, J. Clayden, N. Greeves, S. Warren, and P. Wothers, Oxford University Press, Oxford (2001).
7. *Biological Chemistry*, H.R. Mahler and E.H. Cordes, 2nd Edition, (1971) Harper and Row Pub., New York.
8. *Fundamentals of Biochemistry*, D. Voet, J.G. Voet & CW Pratt, (1999) John Wiley & Sons, New York.



The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The paper consists of following units :

**UNIT - 1 : QUALITATIVE ANALYSIS** 20 marks

Analysis of two metal ions cationic/anionic forms: Cr, Mo, W, V and Mn

**UNIT-2 : QUANTITATIVE ANALYSIS** 30 marks

To analyse quantitatively two constituent ions of the following:

Cu, Zn (b) Ni, Fe (c) Ca, Mg, (d) Al, Mg.

The cations- Mg<sup>2+</sup>, Ca<sup>2+</sup> and Al<sup>3+</sup> can be estimated using EDTA.

**UNIT - 3 : INORGANIC PREPARATION** 20 marks

Pot. trioxalato ferrate (III)

Pot, trioxalato chromate (III)

Diaquo dioxalato chromate (III)

Hexamine Ni (II) chloride

**UNIT - 4 : RECORD** 05 MARKS

**UNIT - 5 : VIVA-VOCE** 25 MARKS

**Books Recommended :**

1. *Vogel's Qualitatives Inorganic Analysis*, revised, Svehla, Orient Longman.
2. *Vogel's Textbook of Qualitatives Inorganic Analysis, (revised)*, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham ELBS.
3. *Standard Methods of Chemical Analysis* W. W. Scott, The Technical Press.
4. *Experimental Inorganic Chemistry*, W. G. Palmer, Cambridge.
5. *Handbook of Preparative Inorganic Chemistry*, Vol.-I & II Brauer, Academic Press.
6. *Inorganic Synthesis*, McGraw Hill.

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## 3<sup>rd</sup> SEMESTER

**PAPER-9**

**MOLECULAR SPECTROSCOPY [CH-301]**

**Marks-70**

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The detailed syllabi will be as follows :

The paper consists of following units :

### UNIT-1 : VIBRATIONAL SPECTROSCOPY

Harmonic oscillator model, Harmonic and anharmonic vibrations, normal vibrations, factors affecting vibrational frequencies, vibrating rotators, P.Q.R., branches, overtones, anharmonic constants, Raman effect, Stokes and Anti-Stokes lines, selection rule for IR and Raman spectra, principle of mutual exclusion, geometry of AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub>, and AB<sub>6</sub> molecules.

Effect of conjugation, resonance, inductive effect, ring strain and hydrogen bonding on group frequencies and band shapes.

Changes with vibrational frequencies upon co-ordination, cases of linkage isomers, metal carbonyls and hydrogen bonding.

### UNIT-2 : UV VISIBLE SPECTROSCOPY

Electronic energy levels, molecular orbitals, Franck London Principle, Different electronic transitions, effect of solvent on electronic transitions, electronic spectra of polyatomic molecules, spectra of carbonyl compounds and conjugated polyenes, Woodward-Feiser rules, spectra of aromatic and heterocyclic compounds.

### UNIT-3 : PHOTOELECTRON SPECTROSCOPY

Basic principles, photoelectric effects, ionization process, PES AND XPS, photoelectron spectra of O<sub>2</sub>, N<sub>2</sub> and NO.

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#### UNIT - 4 : MASS SPECTROMETRY

Ion production and fragmentation, molecular ion peak, meta-stable peak, Mc Lafferty rearrangement, examples of mass spectra of organic compounds.

#### UNIT-5 : MAGNETIC RESONANCE SPECTROSCOPY

Nuclear magnetic resonance, Chemical shift and factors controlling its value, spin-spin interaction and factors affecting its value.

Principles of ESR, presentation of spectrum, theory of hyperfine coupling, Isotropic g and A values. Chemical shift values and correlation for protons bounded with carbon, chemical exchange, coupling constants, interpretation of PMR spectra of organic compounds.

Applications of  $^{19}\text{F}$  and  $^{31}\text{P}$  NMR spectra of inorganic compounds.

#### Books Recommended :

1. *Molecular Structure and spectroscopy*, G. Aruldas, Prentice Hall of India Pvt. Ltd., New Delhi (2001).
2. *Organic Spectroscopy*, W. Kemp, 3rd Edn. (1991), Macmillan, London.
3. *Physical Methods in Chemistry*, R. S. Drago, International Edition (1992), Affiliated East-West Press, New Delhi.
4. *Modern Spectroscopy*, J.M. Hollas, 4th edition (2004), John Wiley and Sons, Chichester.
5. *Fundamentals of Molecular Spectroscopy*, C.N. Banwell and E.M. Mc Cash, 4th edition (1994), Tata McGraw Hill, New Delhi.
6. *Symmetry and Spectroscopy of Molecules*, K. Veera Reddy, New Age International Pvt. Ltd., New Delhi (1999).
7. *Introduction to Magnetic Resonance*, A Carrington and A. D. Mc Lachlan, Chapman and Hall, London (1979).
8. *Nuclear Magnetic Resonance Spectroscopy*, R. K. Harris, Addison Wesley, Longman Ltd, London (1986).
9. *Electronic Absorption Spectroscopy and Related Techniques*, D.N. Sathyanarayana, Universities Press (India) Ltd., Hyderabad (2001).
10. *Introduction to Photoelectron Spectroscopy*, P.K.Ghosh, John Wiley

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The detailed syllabi will be as follows :

The paper consists of following units :

#### UNIT - 1 : METAL IONS IN BIOLOGICAL SYSTEM

Essential and trace metals, Role of metal ions (Ca, Mg, Fe, Na, K) in biological process, metal complexes in transmission of energy Chlorophyll; Photo system-I and Photo system-II in cleavage of water system.

#### UNIT-2 : NATURAL OXYGEN CARRIER

Haemoglobin, Myoglobin, Hemicyanin and hemerythrin. Synthetic oxygen carrier-complex of Cobalt and Iron, Cytochrome-P-450, cytochrome-C, Rubredoxins and ferredoxins, Copper blue proteins, Non Haeme proteins-Ferritin and transferrin, metallozymes, Fixation of Nitrogen. Haeme proteins and oxygen uptake, structure and function of Haemoglobin, myoglobin and hemicyanin.

#### UNIT - 3 : ENZYMES PROPERTIES

Specificity of enzymes, enzyme kinetics, Michalis-Menten equation, steady state kinetics, inhibition, transition state theory, orientation and steric effect; Co-enzymes-cofactors as derived from vitamins, prosthetic groups, thiamine pyrophosphate, pyruvical phosphate, NAD, NADP, FMN, FAD, lipoic acid and Vit. B12.

#### UNIT - 4 : BIOENERGETICS STANDARD

Free energy change in biochemical reactions, hydrolysis of ATP, synthesis of ATP, entropy changes in biological processes.

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## UNIT - 5 : CARBOHYDRATE METABOLISM

Calvin Cycle, Krebs cycle, Glycolysis, Glucogenesis, Glycogenolysis, Gluconogenesis, biosynthesis of disaccharides and polysaccharides, pentose phosphate pathway.

### Books Recommended:

1. *Biochemistry*, L. Stryer, 5th Edition, (2002) Freeman & Co. New York
2. *Biochemistry*, D. Voet, J. G. Voet, 3rd Edition (2004), Wiley International Publication.
3. *Biochemistry*, I. Bertini, H. B. Gray, S. J. Lippard, J.S. Valentine, 1st South Asian Edn., (1998) Viva Books Pvt. Limited, New Delhi .
4. *Principles of Biochemistry*, A.L. Lehninger, (1992) CBS Publishers, Delhi.
5. *Bioorganic Chemistry : A Chemical Approach to Enzyme Action*, H. Dugas and C. Penney, (1981) Springer- Verlag, New York.

## PAPER-11 ENVIRONMENTAL & ANALYTICAL CHEMISTRY [CH-303]

Marks-70

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The detailed syllabi will be as follows :

The paper consists of following units :

### UNIT-1 : WATER POLLUTION

Aquatic pollution-inorganic, organic, pesticide, agricultural, Industrial and Sewage, detergents, oils spills, Water quality parameters-dissolved oxygen, biochemical oxygen demand solid metals, contents of chlorides, sulphates, phosphates, nitrates and macro-organisms, water quality standards. Analytical methods for measuring BOD, DO, COD, F, Oils metals (As, Cd, Cr, Hg, Pb, Se), residual chloride and chlorine demand Purification, and treatment of water.

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## UNIT -2 : ATMOSPHERE

Chemical composition of atmosphere, particles, ions, radicals and their formation, chemicals and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, green house effect, acid rain, air pollution controls and their chemistry, Analytical methods for measuring air pollutants.

## UNIT-3 : INDUSTRIAL POLLUTION

Cement, Sugar, distillery, drug, paper and pulp, thermal power plants, metallurgy, polymers, disposal of industrial waste and their management.

## UNIT-4 : THERMAL ANALYSIS

Basic principles, instrumental methods, quantitative consideration of DTA curve, application. TGA – Basic principles, instrumentation, application, DITG, MDTA.

## UNIT -5 : CHROMATOGRAPHIC TECHNIQUES

Classification, Chromatography terminology (RF Value), development of chromatography, application of chromatographic techniques.

### Books Recommended :

1. *Environmental Chemistry - A Global Perspective*, G. W. Vanloon, S. J. Duffer, Oxford University Press (2000).
2. *Environmental Analytical Chemistry*, F.W. Fifield and W.P.J. Hairens, 2nd Edition (2000), Black Well Science Ltd.
3. *Environmental Chemistry*, Colin Baird, W.H. Freeman and Company, New York (1995).
4. *Environmental Chemistry*, A.K. De, 4th Edition (2000), New Age International Private Ltd., New Delhi.
5. *Analysis of Air Pollutants*, Peter O. Warner, 1st Edition (1996), John Wiley, New York.
6. *Environmental Pollution Analysis*, S.M. Khopkar, 1st Edition (1993), Wiley Eastern Ltd., New Delhi.
7. *Environmental Chemistry*, S.K. Banerji, 1<sup>st</sup> Edition (1993), Prentice-Hall of India, New Delhi.
8. *Principles of Instrumental Analysis*, D.A. Skoog, F.J. Holler and T.A. Nieman, 5th Edition (1998), Saunders College Publishing, Harcourt Brace & Company, U.S.A.
9. *Analytical Chemistry*, G.D. Christian, John Wiley & Sons, New York (2001).
10. *Comprehensive Analytical Chemistry*, C.L. Wilson and D.L. Wilson, Vol. I (A) and I (B), Elsevier.

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**PAPER-12      ORGANIC CHEMISTRY LAB COURSE (GENERAL) [CH-304]**

**Marks-70**

**Unit-1 :** Identification of single compounds using TLC and chemical test.      20 marks

**Unit-2 :** Organic Synthesis (One step Synthesis)      25 marks

**Unit-3 :** Any of the following experiments:      25 marks

Determination of COD & BOD of water sample.

Estimation of amino/phenol-OH using bromated Bromide solution.

Determination of iodine or saponification values of oil.

**Unit-4 :** Note Book      05 marks

**Unit-5 :** Viva-Voce      25 marks

**Books Recommended :**

1. Experimental Organic Chemistry Vol.-I & II, P. R. Singh, D. S. Gupta and K. S. Bajpai, Tata McGraw Hill.
2. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley Eastern.
3. Vogel's Textbook of Practical Organic Chemistry, B. S. Furniss, A. J. Hanaford, V. Rogers, P. W. G. Smith and A. R. Tatchell, ELBS.

Each student has to opt for only one elective subject from the list of the groups offered in 4th semester.

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## 4<sup>th</sup> SEMESTER

### GROUP-A (PHYSICAL CHEMISTRY SPECIALIZATION)

#### PAPER-13 ADVANCED QUANTUM CHEMISTRY [CH-401-P] Marks-70

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The detailed syllabi will be as follows :

The paper consists of following units :

#### UNIT-1 : ELEMENTARY MATRIX THEORY

Review of matrix algebra and angular momentum, projection operator, matrix representation of Schrödinger wave equation, similarity transformation and block diagonalization of matrices, matrix transformation of linear equation.

#### UNIT-2 : GROUP THEORY AND QUANTUM CHEMISTRY

Transformation properties of orbitals, quantitative and qualitative treatments of hybridization scheme involving orbitals. SALC, Formation of group orbital and molecular orbitals, symmetry factorization of secular equation, energy levels and DE in cyclopropene, butadiene, benzene and naphthalene systems.

#### UNIT-3 : HARTREE FOCK THEORY

Born-Oppenheimer approximation, Slater-Codon rules, Hartree-Fock equation, Koopman and Brillouin Theories, Roothan equation, Gaussian basis sets.

#### UNIT-4 : SEMI EMPIRICAL THEORIES

HMO theory of conjugated systems, application to cyclopropane and cyclobutadiene systems, Extended Huckel theory, PPP treatment, ZDO approximation, detailed treatment of CNDO and INDO theories.



theories.

### UNIT-5 : DENSITY FUNCTIONAL THEORY

Derivation of Hohenberg-Kohn theorem, Koln-Sham formulation, N and V-represent abilities, Treatment of chemical concepts with density functional theory.

#### Books Recommended:

1. *Molecular Quantum Mechanics*, P.W. Atkins and R.S. Friedman, 3rd edition (1997), Oxford University Press. Oxford.
2. *Quantum Chemistry*, H. Eyring, J. Walter and G.E. Kimball, John Wiley, New York (1944)
3. *Quantum Chemistry*, I.N. Levine, 5th edition (2000), Pearson Educ., Inc., New Delhi.
4. *Introductory Quantum Chemistry*, A. K. Chandra, 4<sup>th</sup> Edition (1994), Tata Mc-Graw Hill, New Delhi.
5. *Density Functional theory of atoms & Molecules*, Parr & Yang, OUP, Oxford.
6. *Modern Quantum Chemistry*, Ostlund & Szabo, Tata Mc-Graw Hill, New Delhi.

### PAPER-14 AMOLECULAR THERMODYNAMICS [CH-402-P] Marks-70

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The detailed syllabi will be as follows :

The paper consists of following units :

### UNIT-1 : CLASSICAL STATISTICAL MECHANICS

Foundation of molecular thermodynamics ensemble, ensemble average, Liouville theorem, micro-canonical ensemble, canonical and grand canonical ensembles, ideal gas in canonical ensemble, comparison of various ensembles.

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## UNIT-2 : MOLECULAR STATISTICS

Boltzman distribution law of non degenerate and degenerate case, Lagrange method of undetermined multipliers and determination of Boltzman constraints &. Molecular partition function, thermodynamic properties in terms of partition function.

Indistinguishability of identical particles, Bose-Einstein distribution, Fermi-Dirac distribution, degenerate Fermi gas, comparison of M.-B., B. -E. and Fermi Dirac statistics.

## UNIT-3 : MOLECULAR PARTITION FUNCTION

Significance of Boltzman distribution law, separation of partition function, evaluation of translational partition function for ideal monatomic gas, valuation of rotational and vibrational partition function for ideal diatomic and polyatomic gases, electronic and nuclear partition function, statistical interpretation of entropy and heat capacity of gases.

## UNIT-4 : THERMODYNAMICS OF SOLIDS AND LIQUIDS

Specific heat of solids, Einstein heat capacity equation, Debye theory of specific heat, entropy of ortho and para hydrogen and their ratio; Formulation of radial distribution function of liquids and evaluation of various liquids state properties, Florys theory of liquid viscosity.

## UNIT-5 : IRREVERSIBLE THERMODYNAMICS

Microscopic reversibility, entropy flow and entropy production due to irreversible processes inside the system, excess entropy production, local entropy production, generalized thermodynamic forces, thermodynamic fluxes, phenomenological relations, theorem of minimum entropy production.

### Books Recommended:

1. *Introduction of Thermodynamics of irreversible Processes*, I. Prigogine
2. *Thermodynamics For Chemists*, S.Glasstone, Macmillan
3. *Chemical Thermodynamics*, J.A.V.Butler, Macmillan
4. *Physical Chemistry : A Molecular Approach*, D.A. Mc Quarrie and J.D. Simon, (1998) Viva Books, New Delhi.
5. *Statistical Mechanics*, B.K. Agarwal and M. Eisner, Wiley Eastern, New Delhi (1988).
6. *Statistical Mechanics*, D.A. Mcquarrie, Harper and Row Publishers, New York (1976).

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The detailed syllabi will be as follows :

The paper consists of following units :

#### UNIT-1 : KINETICS OF CONDENSED PHASE REACTIONS

Factors determining reaction rate in solution, diffusion controlled reactions and activation controlled reactions, collision on solution encounter, Transition state theory in solution; kinetics of ionic reactions, single and double spherical model, kinetics of dipole-dipole reaction, ion-dipole reactions, dependence of rate constant on ionic strength and dielectric constant of the medium. Bronsted-Bjerrum equation, Primary salt effect, secondary salt effect.

#### UNIT-2 : CATALYSIS AND OSCILLATORY BEHAVIOUR

General mechanism and kinetics of catalytic reactions, Arrhenius intermediates, Van Hoff intermediates, Theory of acid-base catalyst, effect of salt of acid-base catalysis, Bronsted catalysis law, linear free energy relationship, Hammett equation, Oscillatory reactions, Lotka-Volterra model, B-Z reaction and its mechanisms.

#### UNIT-3 : STUDY OF FAST REACTIONS

Flash photolysis, laser Flash Photolysis, relaxation technique, NMR method, Molecular beam and Shock Tube kinetics, stop flow method, laser in photochemical kinetics, Isomerization, Photo dissociation and recombination reactions.

#### UNIT-4 : KINETICS OF ELECTRODE REACTIONS

Faradaic and non-Faradaic current, Rate law in Faradaic process, current density, factors, affecting electrode reaction rate, Nernst diffusion layer treatment, Exchange current density, stoichiometric

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number and transfer coefficient, energy barrier for multistep reactions, effect of double layer structure electrode reaction rates.

### UNIT-5 : ELECTRODE DEPOSITION AND CORROSION PROCESS

Electro-catalysis, electro-catalytic rate, electro-catalysis in redox system, total deposition, current density, time variation of the over potential and rate and rate determining step in electrode deposition, kinetics of corrosion, corrosion current, electronation current and corrosion potential, electronation reaction, corrosion and stability of the metals.

#### Books Recommended:

1. *Reaction Kinetics*, M. J. Pilling and A.P.W, Seakins, Oxford Science Publication, New York (1998).
2. *Chemical Kinetics*, K.J. Laidler, 3rd Edition (1967), Harper & Row Publishers, New York.
3. *Kinetics and Mechanism of Chemical Transformation*, J. Rajaram and J.C. Kuriacose, 1st Edition (1993), MacMillan India Ltd., New Delhi.
4. *Modern Liquid Phase Kinetics*, B. G. Cox, Oxford University Press, Oxford (1994).
5. *Molecular Reaction Dynamics and Chemical Reactivity*, R. D. Levine and R. B. Bernstein, Oxford University Press, Oxford (1987).
6. *Femtochemistry-Ultrafast Dynamics of the Chemical Bond*, A. H. Zewail, Vols. I and II, World Scientific, New Jersey, Singapore (1994).

## PAPER-16 PHYSICAL CHEMISTRY LAB COURSE (SPECIAL)[CH-404-P]

Marks-70

### UNIT-1 : EXPERIMENTS

Two experiments are to be carried out.

35×2 = 70 marks

- ☉ Determination of temperature coefficient and energy of activation of the hydrolysis of ethyl acetate.
- ☉ To determine the rate constant and order of reaction for the reaction between potassium persulphate and potassium iodine and find the temperature coefficient and energy of activation for the reaction.
- ☉ To study the effect of ionic strength of the rate constant for the saponification of an ester.
- ☉ To study the complex formation between  $\text{Cu}^{++}$  and  $\text{NH}_3$  by the distribution method.

- To study the distribution coefficient of iodine between water and CCL<sub>4</sub> and then determine the equilibrium constant for K<sub>1</sub>+I<sub>2</sub> – K<sub>13</sub> by partition method.
- Absorption isotherm for the absorption of acetic acid and oxalic acid on active charcoal by the graphical method.
- Verification of Beer-Lambert Law.
- Determination of water equivalent of calorimeter and heat of displacement for the reaction. :  

$$\text{Cu}^{++} + \text{Zn} = \text{Zn}^{++} + \text{Cu}.$$

UNIT-2 : Note Book

05 marks

UNIT-3: Viva-Voce

25 marks

### Books Recommended:

1. *Experiment Practical Physical Chemistry*, J. B. Yadav, Goel Publishing House.
2. *Advanced Experimental Chemistry*, Vol.-I Physical, J. N. Gurtu and R. Kapoor, S. Chand & Co.
3. *Selected Experiments in Physical Chemistry*, N. G. Mukherjee, J. N. Ghose & Sons.
4. *Experiments in Physical Chemistry*, J. C. Ghose, Bharati Bhawan.

## GROUP-B (INORGANIC CHEMISTRY SPECIALIZATION)

### PAPER-13

### LIGAND FIELD THEORY [CH-401-I]

Marks-70

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees. The paper consists of following units :

#### UNIT-1 : MULTIPLE AND FINE STRUCTURE IN ATOMIC SPECTRA

Free ion terms, Hund's rule, L-S and J-J coupling schemes, Condon and Shortley parameters, Racah

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parameters, Lande internal rules, Multiple separation, spin orbit coupling constant.

### **UNIT-2: METAL ION IN CHEMICAL ENVIRONMENT**

Splitting of terms in Oh and Td and D4h symmetry, Transformation properties of s, p, d, orbitals in a chemical environment by the use of character table, sine formula and its derivatives; strong field configuration, strong field components, Non-crossing rules, correlation diagram for d<sup>2</sup>, d<sup>3</sup>, d<sup>7</sup> and d<sup>8</sup> systems in cubic symmetry, cross over points, T-S diagram.

### **UNIT-3 : M.O. DESCRIPTION FOR BONDING IN CO-ORDINATION COMPOUNDS**

Classification of ligands as sigma- and pi-donor ligands, pi-acceptor ligands, symmetry consideration of metal orbitals and ligand group orbitals in Oh point group for sigma- and pi- M-L bond formation, use of character table for formation of M.Os. in Oh and Td point groups with and without pi- bonding, MO energy level diagram.

### **UNIT-4 : ABSORPTION SPECTRA AND OTHER SPECTROSCOPIC EVIDENCE FOR LIGAND FIELD EFFECT**

Band assignment, determination of ligand field splitting parameters, Nephelauxetic ration, Jahn-Teller distortion, vibronic coupling, spin orbit coupling, CT Bands and their assignments, applications of IR in metal carbonyls, nitrosyls, linkage isomerism, mode of metal ligand bonding.

NMR spectra of paramagnetic transition metal complexes, contact shift, and pseudo contact shift. ESR-principle of ESR spectroscopy, presentation of spectrum, theory of hyperfine interaction, isotopic g and A values, anisotropy, zero field splitting, application to transition metal complexes.

Mossbauer spectra: Mossbauer effect, recoil energy and  $\gamma$ -ray emission, isomer effect, magnetic hyperfine interaction, application of spectra to Fe (57) and Sn (119) compounds.

### **UNIT-5 : MAGNETOCHEMISTRY**

Van Vleck susceptibility equation and its application, TIP effect of spin orbit coupling, magnetic properties of A, E and T ground term complexes, effect of electron demoralization on magnetic property, antiferromagnetic exchange interaction, super exchange interaction and MO theory, low spin and high spin crossover.

#### **Books Recommended:**

1. *Molecular Magnetism*, Oliver Kahn, VCH, Weinheim (1993).
2. *Physical Methods in Inorganic Chemistry*. S. Drago, 1st Edn.(1971), Affiliated East-West Press, New Delhi.
3. *Structural Methods in Inorganic Chemistry*. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.

4. *Chemical Applications of Group Theory*, F. A. Cotton, 3rd Edn. (1999), John Wiley & Sons, New York.
5. *E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock*, Structural Methods in Inorganic Chemistry, 1st Edn. (1987), Blackwell Scientific Publications, Oxford, London.
6. *Introduction to Ligand Fields*, B.N. Figgis, Wiley Eastern Ltd. New Delhi (1976).  
Magnetochemistry, R.L. Carlin, Springer Verlag.

## **PAPER-14 REACTION MECHANISM & SUPRAMOLECULAR CHEMISTRY [CH-402-I]**

**Marks-70**

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees. The paper consists of following units :

### **UNIT-1 : ELECTRON TRANSFER REACTIONS**

Outer sphere and inner sphere mechanism, Marcus-Husch theory, complementary and non-complementary reactions, mixed valence complexes and their electron transfer model.

### **UNIT-2 : MOLECULAR REARRANGEMENT**

D and A process, reaction of geometrical and optical isomers, optical inversions, isomerization and racemisation of octahedral complexes, intramolecular rearrangement.

### **UNIT-3 : PHOTOCHEMISTRY OF METAL COMPLEXES**

Basics of photochemistry, properties of excited states, excited states of metal complexes and their comparisons with organic compounds; photo substitution, photo oxidation and photo reduction, excited electron transfer, reactions of 2,2-bipyridines and 1, 10-Phenanthroline complexes, metal complex sensitizers, photochemistry of Co (III) and Cr (III) complexes, application of photochemical reactions of co-ordination compounds.

## UNIT-4 : SUPRAMOLECULAR CHEMISTRY

Introduction, some examples of metal guided self assembly in supramolecular chemistry, reactivity and catalysis, supramolecular devices

## UNIT-5 : COORDINATION POLYMERS

Synthesis, structure, bonding and application of metal alkoxides, metal acetylacetonates, Schiff base metal complexes.

### Books Recommended:

1. T.C. Bruice and S. Benkovic, *Bioorganic Mechanisms*, Vol. I & II, (1966) W. A. Benjamin, New York.
2. G. J. Ferraudi, *Elements of Inorganic Photochemistry*, John Wiley & Sons (1988).
3. *Supramolecular Chemistry*, Jean-Marie Lehn, VCH, Weinheim (1995).
3. *Chemistry of the Elements*, N. N. Greenwood and A. Earnshaw, 2nd Edn. (1997), Butterworth Heinemann, London.
4. *Principles and Applications of Organotransition metal Chemistry*, J.P. Collman, L.S. Hegeudus, J.R. Norton and R.G. Finke, Univ. Sci. Books, Mill Valley. California
5. *The Organometallic Chemistry of Transition Metals*, R. H. Crabtree, John Wiley.
6. *Photochemistry and Photo-physics of Metal Complexes*, D. M. Roundhill, Plenum Press, New York and London (1994).

## PAPER-15 ORGANOTRANSITION METAL CHEMISTRY & METAL CLUSTERS [CH-403-I]

Marks-70

The theory question paper of every end semester may comprise of long, short and *Objective type questions* covering whole syllabus. The numbers of questions and distribution of marks according to type are as follows:

Type of question	No. of Questions × Marks	Distribution of Marks
Objective Questions	14×2	28
Short Answer Type Questions	7×4	28
Long Answer Type Questions	2×7	14

Four long answer type questions to be set in which two questions to be answered by the examinees.

The paper consists of following units :



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## UNIT-1 : TRANSITION METAL–CARBON $\sigma$ -BOND COMPOUNDS

Introduction to organometallics,  $\sigma$ -alkyl and aryl compounds with transition metals, their synthesis, structure and reactivity, organo-copper in organic synthesis.

## UNIT-2 : TRANSITION METAL $\pi$ -COMPLEXES

Alkene, allyl, alkyne, diene, dienyl, arene and trienyl complexes of transition metals, preparation, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack.

## UNIT-3 : CATALYSIS OF ORGANOMETALLIC COMPOUNDS

Oxidative addition and reductive elimination process, catalytic reactions of olefin-hydrogenation using Wilkinson catalyst, isomerization, hydroformylation (Oxo process and Reppe reaction) by cobalt and Rhodium catalysis, Wacker process, polymerization (Zeigler-Natta process), Oligomerisation, Fischer-Tropsch reaction and water gas reaction, activation of C-H bond.

## UNIT-4 : METAL-METAL BOND AND METAL CLUSTERS

Metal-Metal multiple bonds, major structural type, relation with clusters, one dimensional solids, classification, structure and electron count in M<sub>3</sub>, M<sub>4</sub> and M<sub>5</sub> clusters, LNCC and HNCC structures, Isolobal and isoelectronic relationship.

**UNIT-5 :** Transition metal compounds with bonds to Hydrogen, Encapsulation compounds & Metal-organic frameworks.

### Books Recommended:

1. *Advanced Inorganic Chemistry*, F. A. Cotton and G. Wilkinson, 6th Edn. (1999), John-Wiley & Sons, New York.
2. *Inorganic Chemistry*, James E. Huheey, 4th Edn. (1993), Addison Wesley Pub. Co., New York
3. *Chemistry of the Elements*, N. N. Greenwood and A. Earnshaw, 2<sup>nd</sup> Edn. (1997), Butterworth Heinemann, London.
4. *Inorganic Electronic Spectroscopy*, A.B.P.Lever, Elsevier
5. *Comprehensive Coordination Chemistry*, Wilkinson, Gillars & Mc Cleverty, Pergamon
6. *Transition Metal Chemistry*, R.L.Carlin, vol-3, Dekker.