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Vinayak Ganesh Vaze College of Arts, Science & Commerce  
(AUTONOMOUS)

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The Kelkar Education Trust's  
**Vinayak Ganesh Vaze College of Arts, Science & Commerce**  
**AUTONOMOUS**

Mithagar Road, Mulund East, Mumbai-400081, India  
College with Potential for Excellence  
Phones :022-21631421, 221631423, 221631004 Fax : 022-221634262,  
e mail : vazecollege@gmail.com

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**Syllabus for M. Sc. Part-1 Programme:**

**Chemistry**

Syllabus as per Choice Based Credit System

**(June 2020 Onwards)**

**Submitted by**

**Department of Chemistry**

**Vinayak Ganesh Vaze College of Arts, Science and Commerce**  
Mithagar Road, Mulund ( East) Mumbai-400081. Maharashtra, India.  
Tel: 022-21631004, Fax: 022-21634262

E-mail: [vazecollege@gmail.com](mailto:vazecollege@gmail.com) Website : [www.vazecollege.net](http://www.vazecollege.net)

**Program : M.Sc.**

( Choice Based Credit System )

**Course : M.Sc. Organic Chemistry**

**Part – I**

**Syllabus for Semester I & II**

(To be implemented from the Academic year 2020-2021 )

❖ Syllabus as per Choice Based Credit System

**TOTAL SEMESTERS FOR PART-I : 02**

**CREDIT DISTRIBUTION SEMESTERWISE**

COURSE	PAPER AND SUBJECT	THEORY CREDIT	PRACTICAL CREDIT	TOTAL CREDITS
M.SC – PART-I	<b>PAPER-I</b> PHYSICAL CHEMISTRY	04	02	06
	<b>PAPER-II</b> INORGANIC CHEMISTRY	04	02	06
	<b>PAPER-III</b> ORGANIC CHEMISTRY	04	02	06
	<b>PAPER-IV</b> ANALYTICAL CHEMISTRY	04	02	06
		<b>16</b>	<b>08</b>	<b>24</b>

**Total credits for M.Sc Part-I = 02 X24 =48 credits**

**EVALUATION PATTERN PER PAPER SEMESTERWISE**

THEORY	INTERNALS	PRACTICALS
<b>60</b>	<b>40</b>	<b>50</b>

**INTERNALS INCLUDES PROJECTS/ASSIGNMENTS/TUTORIALS**

**Syllabus for Approval**

<b>Sr. No.</b>	<b>Heading</b>	<b>Particulars</b>
<b>1</b>	<b>Title of Course</b>	<b>M.Sc. Chemistry Semester I and II</b>
<b>2</b>	<b>Eligibility for Admission</b>	The B.Sc. degree examination of this university with chemistry 6 units
<b>3</b>	<b>Passing marks</b>	<b>Minimum D Grade or equivalent minimum marks for passing at the Graduation level.</b>
<b>4</b>	<b>Ordinances/Regulations (if any)</b>	
<b>5</b>	<b>No. of Years/Semesters</b>	<b>One year/Two semester</b>
<b>6</b>	<b>Level</b>	<b>P.G. part-I</b>
<b>7</b>	<b>Pattern</b>	<b>Semester</b>
<b>8</b>	<b>Status</b>	<b>Revised</b>
<b>9</b>	<b>To be implemented from Academic year</b>	<b>2020-2021</b>



- b) Particle in a one, two and three dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels.
- c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy, use of the recursion formula.

[Ref 7, 8 and 9]

### Unit III

#### Chemical Dynamics-I

[15L]

##### Composite Reactions:

Recapitulation: Rate laws, Differential rate equations Consecutive reactions, Steady state Approximation, rate determining steps, Microscopic Reversibility and Detailed Balanced Chain reactions-chain initiation processes. Some inorganic mechanisms: formation and decomposition of phosgene, decomposition of ozone, Reaction between Hydrogen and Bromine and some general examples Organic Decompositions: Decomposition of ethane, decomposition of acetaldehyde Gas phase combustion: Reaction between hydrogen and oxygen, Semenov – Hinshelwood and Thompson mechanism, Explosion limits and factors affecting explosion limits.

Polymerization reactions: Kinetics of stepwise polymerization, Calculation of degree of polymerization for stepwise reaction. Kinetics of free radical chain polymerization, Kinetic chain length and estimation of average no .of monomer units in the polymer produced by chain polymerization.

##### Reaction in Gas Phase

Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kassel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.  
[Ref. 2 and 15, 17, 18]

### Unit IV Electrochemistry [15L]

#### Recapitulation – basics of electrochemistry.

Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and its extension to higher concentration (derivations are expected).

Electrolytic conductance and ionic interaction, relaxation effect,. Debye-Hückel- Onsager equation (derivation expected). Validity of this equation for aqueous and non- aqueous solution, deviations from Onsager equation, Debye -Falkenhagen effect (dispersion of conductance at high frequencies), Wien effect.

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Batteries: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]

Bio-electrochemistry: Introduction, cells and membranes, membrane potentials, theory of membrane potentials, interfacial electron transfer in biological systems, adsorption of proteins onto metals from solution, electron transfer from modified metals to dissolved protein in solution, enzymes as electrodes, electrochemical enzyme-catalysed oxidation of styrene. Goldmann equation. (derivations are expected)

[Ref: 14 and 16, 17, 18]

[Note: Numerical and theoretical problems from each unit are expected]

**References:**

1. Peter Atkins and Julio de Paula, Atkin's *Physical Chemistry*, 7<sup>th</sup> Edn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2<sup>nd</sup> Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3<sup>rd</sup> Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5<sup>th</sup> Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3<sup>rd</sup> Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2<sup>nd</sup> Edn., McMillan and Co. Ltd., London, 1962
7. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
8. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
9. R.K. Prasad, *Quantum Chemistry*, 2<sup>nd</sup> Edn., New Age International Publishers, 2000.
10. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
11. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
12. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
13. Ira N. Levine, *Quantum Chemistry*, 5<sup>th</sup> Edn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
14. Thomas Engel and Philip Reid, *Physical Chemistry*, 3<sup>rd</sup> Edn., Pearson Education Limited 2013.
15. D.N. Bajpai, *Advanced Physical Chemistry*, S. Chand 1<sup>st</sup> Edn., 1992.
16. **Bockris**, John O'M., **Reddy**, Amulya K.N., Gamboa-Aldeco, Maria E., *Modern Electrochemistry*, 2A, Plenum Publishers, 1998.
17. *Physical Chemistry* by Gurtu and Gurtu
18. *A Text book of Physical Chemistry* by K L Kapoor Vol 5 , 2<sup>nd</sup> Edn

**Physical Chemistry Practical**

**Paper I**

**Course Code: PSCHP 101**

**Non – Instrumental:**

1. To determine the heat of solution ( $\Delta H$ ) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperature.
2. To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of  $\text{CaSO}_4$  at room temperature.
3. To investigate the reaction between acetone and iodine.
4. To study the variation in the solubility of  $\text{Ca}(\text{OH})_2$  in presence of  $\text{NaOH}$  and hence to determine the solubility product of  $\text{Ca}(\text{OH})_2$  at room temperature.
5. Graph Plotting of mathematical functions –linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?

**Instrumental:**

1. To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
2. To study the effect of substituent on the dissociation constant of acetic acid conductometrically.
3. To determine  $\text{pK}_a$  values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
4. To verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.

**References:**

- 1 Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
- 2 Practical Physical Chemistry, A.M. James and F.E. Prichard, 3<sup>rd</sup> Edn., Longman Group Ltd., 1974.
- 3 Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.



## Paper II

### Inorganic Chemistry

Course Code: PSCH 102 (60 L)

#### Unit I

##### Chemical Bonding: [15 L]

**Recapitulation of hybridization** Derivation of wave functions for  $sp$ ,  $sp^2$ ,  $sp^3$  orbital hybridization types considering only sigma bonding.

Discussion of involvement of  $d$  orbitals in various types of hybridizations. Concept of resonance, resonance energy derivation expected. Formal charge with examples.

Critical analysis of VBT.

Molecular Orbital Theory for diatomic species of First transition Series.

Molecular Orbital Theory for Polyatomic species considering  $\sigma$  bonding for  $SF_6$ ,  $CO_2$ ,  $B_2H_6$ ,  $I_3^-$  molecular species.

Weak forces of attraction: Hydrogen bonding – concept, types, properties, methods of detection and importance. Van der Waal's forces, ion-dipole, dipole-dipole, London forces.

#### Unit-II

##### Molecular Symmetry and Group Theory: [15L]

Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules.

Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups.

Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations. The Great Orthogonality Theorem and its application in construction of character tables for point groups  $C_{2v}$ ,  $C_{3v}$  and  $D_{2h}$ , structure of character tables.

Applications of Group Theory

- Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in  $AB_n$  (Ammonia,  $CH_4$ ) molecule.
- Determination of symmetry species for translations and rotations.
- Mulliken's notations for irreducible representations.
- Reduction of reducible representations using reduction formula.
- Group-subgroup relationships.
- Descent and ascent in symmetry correlation diagrams showing relationship between different groups.

### Unit-III

#### Materials Chemistry and Nanomaterials: [15 L]

##### Solid State Chemistry

Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.

Structures of Compounds of the type: AB [nickel arsenide (NiAs)], AB<sub>2</sub> [fluorite (CaF<sub>2</sub>) and anti-fluorite structures, rutile (TiO<sub>2</sub>) structure and layer structure [cadmium chloride and iodide (CdCl<sub>2</sub>, CdI<sub>2</sub>)].

Methods of preparation for inorganic solids: Ceramic method, precursor method, sol-gel method (applications in Biosensors), microwave synthesis (discussion on principles, examples, merits and demerits are expected)

##### Nanomaterials

Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett(L-B) method, Biological methods: Synthesis using microorganisms.

Applications in the field of semiconductors, solar cells

### Unit - IV

#### Characterisation of Coordination compounds [15L]

Formation, thermal studies, Conductivity measurements, electronic spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods.

Spectral calculations using Orgel and Tanabe-Sugano diagram, calculation of electronic parameters such as  $\Delta$ , B, C, Nephelauxetic ratio.

Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectral methods.

### References :

#### Unit I

1. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
2. W. W. Porterfield, Inorganic Chemistry-A Unified Approach, 2<sup>nd</sup> Ed., Academic Press, 1993.
3. B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.
4. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Pearson Education Limited, 2<sup>nd</sup> Edition 2005.
5. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, 4<sup>th</sup> Ed., Harper Collins, 1993.

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6. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.

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7. R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The Benjamin Cummings Publishing Company, 1989.
8. G. Miessler and D. Tarr, Inorganic Chemistry, 3<sup>rd</sup> Ed., Pearson Education, 2004.
9. R. Sarkar, General and Inorganic Chemistry, Books & Allied (P) Ltd., 2001.
10. C. M. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 1985.
11. J. N. Murrell, S. F. A. Kettle and J. M. Tedder, The Chemical Bond, Wiley, 1978.
12. G. A. Jeffrey, An Introduction to Hydrogen Bonding, Oxford University Press, Inc., 1997.

#### Unit II

1. F. A. Cotton, Chemical Applications of Group Theory, 2<sup>nd</sup> Edition, Wiley Eastern Ltd., 1989.
2. H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley & Sons, New York, 1996.
3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.
4. K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2<sup>nd</sup> Edition, New Age International Publishers, New Delhi, 2009.
5. A. Salahuddin Kunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2012.
6. P. K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing House. 2014.
7. S. Swarnalakshmi, T. Saroja and R. M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.

#### Unit III

1. Solid State Chemistry Introduction, Lesley E. Smart, Elaine A. Moore, ISBN 0-203-49635-3, Taylor & Francis Group, LLC.
2. Nanomaterials & Nanochemistry, 2007, Catherine Brechignac, Philippe Houdy, Marcel Lahmani, ISBN 978-3-540-72992-1 Springer Berlin Heidelberg New York.
3. Nanomaterials Chemistry, Recent Developments and New Directions C.N.R. Rao, A. Muller, and A.K. Cheetham, ISBN 978-3-527-31664-9, 2007 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
4. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9, Marcel Dekker Inc. New York.
5. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.

6. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-32166-7, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.

#### Unit IV

1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education, 2006.
2. D. Banerjee, Coordination Chemistry
3. Geary Coordination reviews
4. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4<sup>th</sup> ed. Oxford University Press, 2006.
5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6<sup>th</sup> ed. Wiley, 1999,
6. B. Douglas, D. McDaniel and J. Alexander. *Concepts and Models of Inorganic Chemistry*(3rd edn.), John Wiley & Sons (1994).

### Inorganic Chemistry Practical

#### Paper II

#### Course Code: PSCHP 102

#### Inorganic Preparations (Synthesis and Characterization)

- 1) Bis-(tetraethylammonium) tetrachloro Cuprate (II)  $(Et_4 N)_2[CuCl_4]$
- 2) Bis-(tetraethylammonium) tetrachloro Nickelate (II)  $(Et_4 N)_2 [NiCl_4]$
- 3) Bis-(tetraethylammonium) tetrachloro Cobaltate (II)  $(Et_4 N)_2 [CoCl_4]$   
(Any two from above preparations)
- 4) Tetrammine monocarbonyl Cobalt (III) Nitrate  $[Co(NH_3)_4CO_3]NO_3$
- 5) Bis (ethylenediammine) Copper (II) Sulphate  $[Cu(en)_2]SO_4$
- 6) Hydronium dichloro bis( dimethylglyoximate) Cobaltate(III)  $H[Co(dmgh)_2Cl_2]$

#### Instrumentation

- 1) Determination of equilibrium constant by Slope intercept method for  $Fe^{+3}/SCN^-$  system
- 2) Determination of Electrolytic nature of inorganic compounds by Conductance measurement.

#### Reference:

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1<sup>st</sup> Edn., 2010., U.N.Dhur & Sons Pvt Ltd
2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By: Dr Deepak Pant

**Paper III**  
**Organic Chemistry**

**Course Code: PSCH 103 (60 L)**

**Unit I**

**Physical Organic Chemistry: (15 L)**

**Thermodynamic and kinetic requirements of a reaction:** rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, Reactivity vs selectivity, Curtin-Hammett Principle, Microscopic reversibility, Kinetic vs thermodynamic control of organic reactions.

**Determining mechanism of a reaction:** Product analysis, kinetic studies, use of isotopes (Kinetic isotope effect – primary and secondary kinetic isotope effect). Detection and trapping of intermediates, crossover experiments and stereochemical evidence.

**Acids and Bases:** Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation. Comparative study of acidity and basicity of organic compounds on the basis of pKa values, Leveling effect and non-aqueous solvents. Acid and base catalysis – general and specific catalysis with examples.

*[Reference Books: 1, 2, 3, 16]*

**Unit II**

**Nucleophilic substitution reactions and Aromaticity**

**Nucleophilic substitution reactions: (9 L)**

**Aliphatic nucleophilic substitution:** S<sub>N</sub>1, S<sub>N</sub>2, S<sub>N</sub><sup>i</sup> reactions, mixed S<sub>N</sub>1 and S<sub>N</sub>2 and SET mechanisms. S<sub>N</sub> reactions involving NGP - participation by aryl rings, α- and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. S<sub>N</sub>CA, S<sub>N</sub>1<sup>o</sup> and S<sub>N</sub>2<sup>o</sup> reactions. S<sub>N</sub> at sp<sup>2</sup> (vinylic) carbon.

**Aromatic nucleophilic substitution:** S<sub>N</sub>Ar, S<sub>N</sub>1, benzyne mechanisms. Ipso, cine, tele and vicarious substitution.

**Ester hydrolysis:** Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.

**Aromaticity:** (6 L)

**Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.**

Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel's  $(4n+2)$  and  $4n$  rules.

Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene ( $C_{60}$ ).

[Reference Books: 4-15]

**Unit-III Stereochemistry:** (15)

**Concept of Chirality:** Recognition of symmetry elements.

**Molecules with tri- and tetra-coordinate centers:** Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities.

**Molecules with two or more chiral centers:** Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Interconversion of Fischer, Sawhorse, Newman and Flying wedge projections. Constitutionally symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereogenic, chirotopic, and pseudoasymmetric centres. R-S nomenclature for chiral centres in acyclic and cyclic compounds.

**Axial and planar chirality:** Principles of axial and planar chirality. Stereochemical features and configurational descriptors (R,S) for the following classes of compounds: allenes, alkylidene cycloalkanes, spirans, biaryls (buttressing effect) (including BINOLs and BINAPs), ansa compounds, cyclophanes, trans-cyclooctenes.

**Prochirality:** Chiral and prochiral centres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotopic and diastereotopic) ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereoheterotopic ligands and faces. Symbols for stereoheterotopic ligands in molecules with i) one or more prochiral centres ii) a chiral as well as a prochiral centre, iii) a prochiral axis iv) a prochiral plane v) pro-pseudoasymmetric centre. Symbols for enantiotopic and diastereotopic faces.

[Reference Books: 6-8]

#### Unit-IV

**Oxidation and Reduction:** (15 L)

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**Oxidation:** General mechanism, selectivity, and important applications of the following:



**Dehydrogenation:** Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).

**Oxidation of alcohols to aldehydes and ketones:** Chromium reagents such as  $K_2Cr_2O_7/H_2SO_4$  (Jones reagent),  $CrO_3$ -pyridine (Collin's reagent), PCC (Corey's reagent) and PDC (Cornforth reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Corey-Kim oxidation - advantages over Swern and limitations; and Pfitzner-Moffatt oxidation-DCC and DMSO and Oppenauer oxidation.

**Oxidation involving C-C bonds cleavage:** Glycols using  $HIO_4$ ; cycloalkanones using  $CrO_3$ ; carbon-carbon double bond using ozone,  $KMnO_4$ ,  $CrO_3$ ,  $NaIO_4$  and  $OsO_4$ ; aromatic rings using  $RuO_4$  and  $NaIO_4$ .

**Oxidation involving replacement of hydrogen by oxygen:** oxidation of  $CH_2$  to  $CO$  by  $SeO_2$ , oxidation of arylmethanes by  $CrO_2Cl_2$  (Etard oxidation).

**Oxidation of aldehydes and ketones:** with  $H_2O_2$  (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)

**Reduction:** General mechanism, selectivity, and important applications of the following reducing reagents:

**Reduction of CO to  $CH_2$  in aldehydes and ketones-** Clemmensen reduction, Wolff- Kishner reduction and Huang-Minlon modification.

**Metal hydride reduction:** Boron reagents ( $NaBH_4$ ,  $NaCNBH_3$ , diborane, 9-BBN,  $Na(OAc)_3BH$ , aluminium reagents ( $LiAlH_4$ , DIBAL-H, Red Al, L and K- selectrides).

$NH_2NH_2$  (diimide reduction) and other non-metal based agents including organic reducing agents (Hantzsch dihydropyridine).

**Dissolving metal reductions:** using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid  $NH_3$  mediated reduction (Birch reduction) of aromatic compounds and acetylenes.

[Reference Books: 17, 18, 14]

#### Reference Books:

1. Physical Organic Chemistry, Neil Isaacs
2. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty
3. Comprehensive Organic chemistry, Barton and Ollis, Vol 1
4. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
5. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.
6. Stereochemistry: Conformation and mechanism, P.S. Kalsi, New Age International, New Delhi.
7. Stereochemistry of carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Manden, Wiley.

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8. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. New International Publishers Ltd.
9. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
10. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
11. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
12. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
13. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
14. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.
15. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
16. Mechanism in Organic Chemistry, Peter sykes, 6th edition onwards.
17. Modern Methods of Organic Synthesis, W. Carruthers and Iain Coldham, Cambridge University Press.
18. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, Pragati Prakashan.

**Organic Chemistry Practical Paper**

**III**

**Course Code: PSCHP 103**

**One step preparations (1.0 g scale)**

1. Bromobenzene to p-nitrobromobenzene
2. Anthracene to anthraquinone
3. Benzoin to benzil
4. Anthracene to Anthracene maleic anhydride adduct
5. 2-Naphthol to BINOL
6. p-Benzoquinone to 1,2,4-triacetoxybenzene
7. Ethyl acetoacetate to 3-methyl-1-phenylpyrazol-5-one
8. o-Phenylenediamine to 2-methylbenzimidazole
9. o-Phenylenediamine to 2,3-diphenylquinoxaline
10. Urea and benzil to 5,5-diphenylhydantoin

**Learning points:**

1. Planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS should be learnt.
2. Purify the product by crystallization. Formation and purity of the product should be checked by TLC
3. Report mass and melting point of the purified product.

## Paper IV

### Analytical Chemistry

#### Unit - I

**Course Code: PSCH 104**

**(60 L)**

#### **Language of Analytical Chemistry**

**[8 L]**

Analytical perspective, Common analytical problems, terms involved in analytical chemistry (analysis, determination, measurement, techniques, methods, procedures and protocol)

An overview of analytical methods, types of instrumental methods, instruments for analysis, data domains, electrical and non-electrical domains, detectors, transducers and sensors, selection of an analytical method, accuracy, precision, selectivity, sensitivity, detection limit and dynamic range.

Errors, determinate and indeterminate errors. Types of determinate errors, tackling of errors.

Quantitative methods of analysis: calibration curve, standard addition and internal standard method.

#### **Quality in Analytical Chemistry:**

**[7 L]**

##### **Quality Management System (QMS):**

Evolution and significance of Quality Management, types of quality standards for laboratories, total quality management (TQM), philosophy implementation of TQM (reference of Kaizen, Six Sigma approach & 5S), quality audits and quality reviews, responsibility of laboratory staff for quality and problems.

##### **Safety in Laboratories:**

Basic concepts of Safety in Laboratories, Personal Protection Equipment (PPE), OSHA, Toxic Hazard (TH) classifications, Hazardous Chemical Processes (including process calorimetry / thermal build up concepts).

##### **Accreditations:**

Accreditation of Laboratories, Introduction to ISO series, Indian Government Standards (ISI, Hallmark, Agmark)

##### **Good Laboratory Practices (GLP)**

Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score

#### Unit- II

#### **Calculations based on Chemical Principles**

**[15 L]**

**The following topics are to be covered in the form of numerical problems only.**

- Concentration of a solution based on volume and mass units.
- Calculations of ppm, ppb and dilution of the solutions, concept of mmol.

- c. Stoichiometry of chemical reactions, concept of kg mol, limiting reactant, theoretical and practical yield.
- d. Solubility and solubility equilibria, effect of presence of common ion.
- e. Calculations of pH of acids, bases, acidic and basic buffers.
- f. Concept of formation constants, stability and instability constants, stepwise formation constants.
- g. Oxidation number, rules for assigning oxidation number, redox reaction in term of oxidation number, oxidizing and reducing agents, equivalent weight of oxidizing and reducing agents, stoichiometry of redox titration (Normality of a solution of a oxidizing / reducing agent and its relationship with molarity).

### Unit III

**Optical Methods** [15 L]

**Recapitulation and FT Technique** [3 L]

Recapitulation of basic concepts, Electromagnetic spectrum, Sources, Detectors, sample containers.

Laser as a source of radiation, Fibre optics

Introduction of Fourier Transform

**Molecular Ultraviolet and Visible Spectroscopy** [6 L]

NUMERICALS ARE EXPECTED

Derivation of Beer- Lambert's Law and its limitations, factors affecting molecular absorption, types of transitions [emphasis on charge transfer absorption], pH, temperature, solvent and effect of substituents.

Applications of Ultraviolet and Visible spectroscopy:

- 1) On charge transfer absorption
- 2) Simultaneous spectroscopy
- 3) Derivative Spectroscopy

Dual spectrometry – Introduction, Principle, Instrumentation and Applications

**Infrared Absorption Spectroscopy** [6 L]

Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument **05 L**

FTIR and its advantages

Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on "Finger print" region, Quantitative analysis, Advantages and Limitations of IR

Introduction and basic principles of diffuse reflectance spectroscopy.

#### Unit - IV

**Thermal Methods:** **[9 L]**

**Introduction,** Recapitulation of types of thermal methods, comparison between TGA and DTA.

**Differential Scanning Calorimetry-** Principle, comparison of DTA and DSC, Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting curves (sample size, sample shape, pressure).

**Applications** - Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage crystallinity, oxidative stability, Drug analysis, Magnetic transition. e.g. Analysis of Polyethylene for its crystallinity.

**Automation in chemical analysis:** **[6 L]**

Need for automation, Objectives of automation, An overview of automated instruments and instrumentation, process control analysis, flow injection analysis, discrete automated systems, automatic analysis based on multilayered films, gas monitoring equipments, Automatic titrators.

#### References Unit I

1. Modern Analytical Chemistry by David Harvey, McGraw-Hill Higher Education
2. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5<sup>th</sup> Edition, Ch: 1.
3. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9<sup>th</sup> Edition, 2004, Ch: 5.
4. Undergraduate Instrumental Analysis, 6<sup>th</sup> Edition, J W Robinson, Marcel Dekker, Ch:1.
5. ISO 9000 Quality Systems Handbook, Fourth Edition, David Hoyle. (Chapter: 3 & 4) (Free download).
6. Quality in the Analytical Laboratory, Elizabeth Pichard, Wiley India, Ch: 5, Ch: 6 & Ch: 7.
7. Quality Management, Donna C S Summers, Prentice-Hall of India, Ch:3.
8. Quality in Totality: A Manager's Guide To TQM and ISO 9000, ParagDiwan, Deep & Deep Publications, 1st Edition, 2000.
9. Quality Control and Total Quality Management - P.L. Jain-Tata McGraw-Hill (2006)  
Total Quality Management - Bester field - Pearson Education, Ch:5.
10. Industrial Hygiene and Chemical Safety, M H Fulekar, Ch:9, Ch:11 & Ch:15.
11. Safety and Hazards Management in Chemical Industries, M N Vyas, Atlantic Publisher, Ch:4, Ch:5 & Ch:19.
12. Staff, World Health Organization (2009) Handbook: Good Laboratory Practice (GLP)
13. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications. OECD. 1. 1998.
14. Klimisch, HJ; Andreae, M; Tillmann, U (1997). "A systematic approach for evaluating the quality of experimental toxicological and eco-toxicological data". doi:10.1006/rtph.1996.1076. PMID 9056496.

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### Unit II

1. 3000 solved problems in chemistry, Schaums Solved problem series, David E. Goldbers, Mc Graw Hill international Editions, Chapter 11,15,16,21,22

### Unit III

1. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5<sup>th</sup> Edition, Harcourt Asia Publisher. Chapter 6, 7.
2. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, 6<sup>th</sup> Edition, CBS Publisher. Chapter 2.
3. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 8.
4. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5<sup>th</sup> Edition, Harcourt Asia Publisher. Chapter 13, 14.
5. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, 6<sup>th</sup> Edition, CBS Publisher. Chapter 2.
6. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 5.
7. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5<sup>th</sup> Edition, McGraw Hill Publisher, Chapter 3.
8. M. Ito, The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding, J. Mol. Spectrosc. 4 (1960) 106-124.
9. A. J. Somnessa, The effect of temperature on the visible absorption band of iodine in several solvents, Spectrochim. Acta. Part A: Molecular Spectroscopy, 33 (1977) 525-528.
10. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5<sup>th</sup> Edition, Harcourt Asia Publisher. Chapter 16, 17.
11. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 12
12. Z. M. Khoshhesab (2012). Infrared Spectroscopy- Materials Science, Engineering and Technology. Prof. Theophanides Theophile (Ed.). ISBN: 978-953- 51-0537- 4, InTech,(open access)

### Unit IV

1. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27
2. Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications
3. Instrumental methods of analysis, 7<sup>th</sup> Edition, Willard, Merrit, Dean: Chapter 25
4. Instrumental Analysis, 5<sup>th</sup> Edition, Skoog, Holler and Nieman: Chapter 31
5. Quantitative Chemical Analysis, 6<sup>th</sup> Edition, Vogel: Chapter 12
6. Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd & Kenneth H. Tonge
7. Instrumental methods of analysis, 7<sup>th</sup> Edition, Willard, Merrit, Dean: Chapter 26
8. Instrumental Analysis, 5<sup>th</sup> Edition, Skoog, Holler and Nieman: Chapter 33
9. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. GrawHill (1987): Chapter 28

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Analytical Chemistry Practical

Paper IV

Course Code: PSCHP 104

1. To carry out assay of the sodium chloride injection by Volhard's method.  
Statistical method.
2. To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.
3. To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.
4. To determine the breakthrough capacity of a cation exchange resin.
5. To determine the lead and tin content of a solder alloy by titration with EDTA.
6. To determine amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).
7. To determine number of nitro groups in the given compound using  $TiCl_3$ .

References:

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogel, 3<sup>rd</sup> Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas, Pearson education
3. Standard methods of chemical analysis, F. J. Welcher
4. Standard Instrumental methods of Chemical Analysis, F. J. Welcher
5. W.W.Scott."Standard methods of Chemical Analysis",Vol.I, Van Nostrand Company,Inc.,1939.
6. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals",Part-II,4th Ed.,A Wiley Interscience Publication,New York,1978.

## Semester – II

### Paper I

#### Physical Chemistry: Course Code: PSCH 201 [60 L]

##### Unit – 1 Chemical Thermodynamics II [15 L]

Fugacity of real gases, Determination of fugacity of real gases using graphical method and from equation of state. Equilibrium constant for real gases in terms of fugacity. Gibbs energy of mixing, entropy and enthalpy of mixing.

**Real solutions:** Chemical potential in non ideal solutions excess functions of non ideal solutions calculation of partial molar volume and partial molar enthalpy, Gibbs Duhem Margules equation.

**Thermodynamics of surfaces,** Pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).

Bioenergetics : standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

##### Unit II

##### Quantum Chemistry II [15 L]

Rigid rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the  $\phi$  equation, wavefunction, quantum number, the  $\theta$  equation, wave function, quantization of rotational energy, spherical harmonics.

Hydrogen atom, the two particle problem, separation of the energy as translational and potential, separation of variables, the  $R$  the  $\phi$  \* and the  $\theta$  equations, solution of the equation, introduction of the four quantum numbers and their interdependence on the basis of the solutions of the three equations, total wave function, expression for the energy, probability density function, distances and energies in atomic units, radial and angular plots., points of maximum probability, expressions for the total wave function for 1s, 2s, 2p and 3d orbitals of hydrogen.

Application of the Schrödinger equation to two electron system, limitations of the equation, need for the approximate solutions, methods of obtaining the approximate



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solution of the Schrödinger wave equation.

Hückel Molecular Orbitals theory for ethylene , 1,3-butadiene and benzene.

*(Derivation expected)*

### Unit III

#### Chemical Kinetics and Molecular Reaction Dynamics

[15 L]

**Elementary Reactions in Solution:-** Solvent Effects on reaction rates, Reactions between ions- influence of solvent Dielectric constant, influence of ionic strength, Linear free energy relationships Enzyme action

**Kinetics of reactions catalyzed by enzymes** -Michaelis-Menten analysis, Lineweaver-Burk and Eadie Analyses.

**Inhibition of Enzyme action:** Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.

**Kinetics of reactions in the Solid State:-** Factors affecting reactions in solids **Rate laws for reactions in solid:** The parabolic rate law, The first order rate Law, the contracting sphere rate law, Contracting area rate law, some examples of kinetic studies.

(Ref: 7 and 2)

### Unit IV

#### Solid State Chemistry and Phase Equilibria

[15 L]

##### : Solid State Chemistry

**Recapitulation:** Structures and Defects in solids.

##### Types of Defects and Stoichiometry

- Zero dimensional (point) Defects
- One dimensional (line) Defects
- Two dimensional (Planar) Defects
- Thermodynamics of formation of defects (Mathematical derivation to find concentration of defects and numerical problems based on it)

(Ref: 17, 18 and 19 )

##### Phase equilibria

**Recapitulation:** Introduction and definition of terms involved in phase rule. Thermodynamic derivation of Gibbs Phase rule.

##### Two component system:

- Solid –Gas System : Hydrate formation, Amino compound formation
- Solid – Liquid System: Formation of a compound with congruent melting point, Formation of a compound with incongruent melting point . (with suitable examples)

##### Three component system

Type-I : Formation of one pair of partially miscible liquids

Type-II: Formation of two pairs of partially miscible liquids

Type-III: Formation of three pairs of partially miscible liquids

(Ref: 4, 6, 11, 12 ,13,16, 24 )

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## References

1. Peter Atkins and Julio de Paula, *Atkins's Physical Chemistry*, 7<sup>th</sup> Edn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2<sup>nd</sup> Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3<sup>rd</sup> Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5<sup>th</sup> Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3<sup>rd</sup> Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2<sup>nd</sup> Edn., McMillan and Co. Ltd., London, 1962.
7. Principles of Chemical Kinetics, 2<sup>nd</sup> Ed., James E. House, ELSEVIER, 2007.
8. B.K. Sen, *Quantum Chemistry including Spectroscopy*, Kalyani Publishers, 2003.
9. A.K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw – Hill, 1994.
10. R.K. Prasad, *Quantum Chemistry*, 2<sup>nd</sup> Edn., New Age International Publishers, 2000.
11. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
12. W.G. Davis, *Introduction to Chemical Thermodynamics – A Non – Calculus Approach*, Saunders, Philadelphia, 19772.
13. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
14. Ira N. Levine, *Quantum Chemistry*, 5<sup>th</sup> Edn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
15. Thomas Engel and Philip Reid, *Physical Chemistry*, 3<sup>rd</sup> Edn., Pearson Education Limited 2013.
16. D.N. Bajpai, *Advanced Physical Chemistry*, S. Chand 1<sup>st</sup> Edn., 1992.
17. Solid State Chemistry [An Introduction], 3rd Ed., Lesley E. Smart & Elaine A. Moore, Taylor & Francis, 2010.
18. The Physics and „Chemistry of Solids, Stephen Elliott, Willey India, 2010
19. Principles of the Solid State, H.V. Keer, New Age International Publishers, 2011.
20. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers, 1996.
21. Principles of physical Chemistry , Marrown and Prutton 5<sup>th</sup> edition
22. Essentials of Physical Chemistry , Arun Bahl, B. S Bahl, G. D.Tulli , S Chand and Co. Ltd , 2012 Edition.
23. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
24. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd ,2011
25. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan , Cambridge University Press.

Physical Chemistry Practical Paper I

Course Code: PSCHP 201

**Non – instrumental:**

1. Polar plots of atomic orbitals such as  $1s$ ,  $2p$  and  $3d$  orbitals by using angular part of hydrogen atom wave functions.
2. To study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate.
3. To study phase diagram of three component system water – chloroform /toluene - acetic acid.
4. To determine the rate constant of decomposition reaction of diacetone alcohol by dilatometric method.

**Instrumental:**

1. To determine the formula of silver ammonia complex by potentiometric method.
2. To determine CMC of sodium Lauryl Sulphate from measurement of conductivities at different concentrations.
3. To determine Hammett constant of *m*- and *p*- amino benzoic acid/nitro benzoic acid by pH measurement.
4. To determine the Michaelis – Menten's constant value ( $K_m$ ) of the enzyme Beta Amylase spectrophotometrically.

**References**

- 4 Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
- 5 Practical Physical Chemistry, A.M. James and F.E. Prichard, 3<sup>rd</sup> Edn., Longman Group Ltd., 1974.
- 6 Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

Semester II Paper II

**Inorganic Chemistry: Course Code: PSCH 202**

**Unit I**

**Inorganic Reaction Mechanism: [15 L]**

Rate of reactions, factors affecting the rate of reactions, techniques for determination of rate of reaction (Direct chemical analysis, spectrophotometric method, electrochemical and flow methods).

Ligand substitution reactions of:

- Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method)
- Square planar complexes, trans-effect, its theories and applications. Mechanism and factors affecting these substitution reactions.

Redox reactions: inner and outer sphere mechanisms, complimentary and non-complimentary reactions.

Stereochemistry of substitution reactions of octahedral complexes. (Isomerization and racemization reactions and applications.)

**Unit II**

**Organometallic Chemistry of Transition metals: [15 L]**

Eighteen and sixteen electron rule and electron counting with examples.

Preparation and properties of the following compounds

- Alkyl and aryl derivatives of Pd and Pt complexes
  - Carbenes and carbynes of Cr, Mo and W
  - Alkene derivatives of Pd and Pt
  - Alkyne derivatives of Pd and Pt
  - Allyl derivatives of nickel
  - Sandwich compounds of Fe, Cr and Half Sandwich compounds of Cr, Mo.
- 2.3 Structure and bonding on the basis of VBT and MOT in the following organometallic compounds:

Zeise's salt, bis(triphenylphosphine)diphenylacetylene platinum(0)  
 $[\text{Pt}(\text{PPh}_3)_2(\text{HC}\equiv\text{CPh})_2]$ , diallylnickel(II), ferrocene and bis(arene)chromium(0),  
tricarbonyl ( $\eta^2$ -butadiene) iron(0).

**Unit III**

**Environmental Chemistry:[15 L]**

**Conception of Heavy Metals:** Critical discussion on heavy metals

**Toxicity of metallic species:** Mercury, lead, cadmium, arsenic, copper and chromium, with respect to their sources, distribution, speciation, biochemical effects and toxicology, control and treatment.

**Case Studies:**

- (a) Itai-itai disease for Cadmium toxicity,
- (b) Arsenic Poisoning in the Indo-Bangladesh region.

**Interaction of radiation in context with the environment:** Sources and biological implication of radioactive materials. Effect of low level radiation on cells- Its applications in diagnosis and treatment, Effect of radiation on cell proliferation and cancer.

**Unit IV**

**Bioinorganic Chemistry:[15 L]**

Biological oxygen carriers; hemoglobin, hemerythrin and hemocyanin- structure of metal active center and differences in mechanism of oxygen binding, Differences between hemoglobin and myoglobin: Cooperativity of oxygen binding in hemoglobin and Hill equation, pH dependence of oxygen affinity in hemoglobin and myoglobin and its implications.

Activation of oxygen in biological system with examples of mono-oxygenases, and oxidases- structure of the metal center and mechanism of oxygen activation by these enzymes.

Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site

Nitrogen fixation-nitrogenase, hydrogenases

Metal ion transport and storage: Ionophores, transferrin, ferritin and metallothioneins

Medicinal applications of cis-platin and related compounds

**References**

**Unit I**

1. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5<sup>th</sup> Ed., Oxford University Press, 2010.
2. D. Banerjee, Coordination Chemistry, Tata McGraw Hill, 1993.
3. W. H. Malik, G. D./ Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8<sup>th</sup> Ed., S. Chand & Company Ltd.
4. M. L. Tobe and J. Burgess, Inorganic Reaction Mechanism, Longman, 1999.
5. S. Asperger, Chemical kinetics and Inorganic Reaction Mechanism, 2<sup>nd</sup> Ed., Kluwer Academic/ Plenum Publishers, 2002
6. Gurdeep Raj, Advanced Inorganic Chemistry-Vol.II, 12<sup>th</sup> Edition, Goel publishing house, 2012.

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7. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
8. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2<sup>nd</sup> Ed., Wiley, 1967.
9. R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001.
10. Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3<sup>rd</sup> Ed., Oxford University Press 2008.

#### Unit II

1. D. Banerjea, Coordination chemistry. Tata McGraw Hill, New Delhi, 1993.
2. R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2<sup>nd</sup>ed, New Age International Pvt Ltd, 2000.
3. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5<sup>th</sup> edition, Wiley International Pvt, Ltd 2000.
4. B.Doughlas, D.H McDaniel and J.J Alexander. Concepts and Models of Inorganic Chemistry, 2<sup>nd</sup> edition, John Wiley and Sons. 1983.
5. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.

#### Unit III

1. Environmental Chemistry 5<sup>th</sup> edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.
2. Environmental Chemistry 7<sup>th</sup> edition, Stanley E. Manahan, CRC Press Publishers,
3. Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.
4. Environmental Science 13<sup>th</sup> edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN-10: 0-495-56016-2, Brooks/Cole, Cengage Learning, 2010.
5. Fundamentals of Environmental and Toxicological Chemistry 4<sup>th</sup> edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor & Francis Group, 2013.
6. Living in the Environment 17<sup>th</sup> edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN-10: 0-538-49414-X, Brooks/Cole, Cengage Learning, 2011
7. Poisoning and Toxicology Handbook, Jerrold B. Leikin, Frank P. Paloucek, ISBN: 1-4200-4479-6, Informa Healthcare USA, Inc.
8. Casarett and Doull's Toxicology- The Basic Science of Poisons 6<sup>th</sup> edition, McGraw-Hill, 2001.

#### Unit IV

1. R. W. Hay, *Bioinorganic Chemistry*, Ellis Harwood, England, 1984.
2. I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, First South Indian Edition, Viva Books, New Delhi, 1998.

3. J. A. Cowan, *Inorganic Biochemistry-An introduction*, VCH Publication, 1993.
4. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Publications, Mill Valley, Caligronic, 1994.
5. G.N. Mukherjee and A. Das, *Elements of Bioinorganic Chemistry*, Dhuri & Sons, Calcutta, 1988.
6. J.Chem. Educ. (Special issue), Nov, 1985.
7. E.Frienden, J.Chem. Educ., 1985, 62.
8. Robert R.Crechton, *Biological Inorganic Chemistry – An Introduction*, Elsevier
9. J. R. Frausto da Silva and R. J. P. Williams *The Biological Chemistry of the Elements*, Clarendon Press, Oxford, 1991.
10. JM. D. Yudkin and R. E. Offord *A Guidebook to Biochemistry*, Cambridge University Press, 1980.

**Inorganic Chemistry Practical  
Paper II**

**Course Code: PSCHP 202**

**Ores and Alloys**

- 1) Analysis of Devarda's alloy
- 2) Analysis of Cu – Ni alloy
- 3) Analysis of Tin Solder alloy
- 4) Analysis of Limestone.

**Instrumentation**

- 1) Estimation of Copper using Iodometric method Potentiometrically.
- 2) Estimation of  $\text{Fe}^{+3}$  solution using  $\text{Ce(IV)}$  ions Potentiometrically

**Reference:**

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1<sup>st</sup> Edn., 2010., U.N.Dhur & Sons Pvt Ltd
2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By: Dr Deepak Pant



**Paper III**

**Organic Chemistry: Course Code: PSCH 203**

**Lectures 60 L**

**Unit-I**

**Alkylation of Nucleophilic Carbon Intermediates: (7 L)**

Generation of carbanion, kinetic and thermodynamic enolate formation, Regioselectivity in enolate formation, alkylation of enolates.

Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site of alkylation.

Alkylation of aldehydes, ketones, esters, amides and nitriles.

Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines and imines.

Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).

**Reaction of carbon nucleophiles with carbonyl groups: (8 L)**

Mechanism of Acid and base catalyzed Aldol condensation, Mixed Aldol condensation with aromatic aldehydes, regiochemistry in mixed reactions of aliphatic aldehydes and ketones, intramolecular Aldol reaction and Robinson annulation.

Addition reactions with amines and iminium ions; Mannich reaction.

Amine catalyzed condensation reaction: Knoevenagel reaction.

Acylation of carbanions.

[Reference Books: 1-11]

**Unit II**

**Reactions and Rearrangements: (15 L)**

Mechanisms, stereochemistry (if applicable) and applications of the following:

**Reactions:** Baylis-Hilman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction.

**Concerted rearrangements:** Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton-Katritzky.

**Cationic rearrangements:** Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.

**Anionic rearrangements:** Brook, Neber, Von Richter, Wittig, Gabriel-Colman, Payne.

[Reference Books: 19-22]

### Unit-III

#### **Introduction to Molecular Orbital Theory for Organic Chemistry: ( 7 L)**

**Molecular orbitals:** Formation of  $\sigma$ - and  $\pi$ -MOs by using LCAO method. Formation of  $\pi$  MOs of ethylene, butadiene, 1, 3, 5-hexatriene, allyl cation, anion and radical. Concept of nodal planes and energies of  $\pi$ -MOs

**Introduction to FMOs:** HOMO and LUMO and significance of HOMO-LUMO gap in absorption spectra as well as chemical reactions. MOs of formaldehyde: The effect of electronegativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO ( $\pi$  and  $\pi^*$  orbitals) of formaldehyde. A brief description of MOs of nucleophiles and electrophiles. Concept of „donor-acceptor“ interactions in nucleophilic addition reactions on formaldehyde. Connection of this HOMO-LUMO interaction with „curved arrows“ used in reaction mechanisms. The concept of hardness and softness and its application to electrophiles and nucleophiles. Examples of hard and soft nucleophiles/ electrophiles. Identification of hard and soft reactive sites on the basis of MOs.

Application of FMO concepts in (a)  $S_N^2$  reaction, (b) Lewis acid base adducts ( $BF_3-NH_3$  complex), (c) ethylene dimerization to butadiene, (d) Diels-Alder cycloaddition, (e) regioselective reaction of allyl cation with allyl anion (f) addition of hydride to formaldehyde.

#### **Applications of UV and IR spectroscopy: (8 L)**

**Ultraviolet spectroscopy:** Recapitulation, UV spectra of dienes, conjugated polyenes (cyclic and acyclic), carbonyl and unsaturated carbonyl compounds, substituted aromatic compounds. Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, and solvent polarity. Calculation of absorption maxima for above classes of compounds by Woodward-Fieser rules (using Woodward-Fieser tables for values for substituents).

**Infrared spectroscopy:** Fundamental, overtone and combination bands, vibrational coupling, factors affecting vibrational frequency (atomic weight, conjugation, ring size, solvent and hydrogen bonding). Characteristic vibrational frequencies for alkanes, alkenes, alkynes, aromatics, alcohols, ethers, phenols, amines, nitriles and nitro compounds. Detailed study of vibrational frequencies of carbonyl compounds, aldehydes, ketones, esters, amides, acids, acid halides, anhydrides, lactones, lactams and conjugated carbonyl compounds.

### Unit-IV **NMR spectroscopy and Mass spectrometry (15 L)**

**Proton magnetic resonance spectroscopy:** Principle, Chemical shift, Factors affecting chemical shift (Electronegativity, H-bonding, Anisotropy effects). Chemical and magnetic equivalence, Chemical shift values and correlation for protons bonded to carbon and other nuclei as in alcohols, phenols, enols, carboxylic acids, amines, amides. Spin-spin coupling, Coupling constant (J), Factors affecting J, geminal, vicinal and long range coupling (allylic and aromatic). First order spectra, Karplus equation.

**$^{13}\text{C}$  NMR spectroscopy:** Theory and comparison with proton NMR, proton coupled and decoupled spectra, off-resonance decoupling. Factors influencing carbon shifts, correlation of chemical shifts of aliphatic, olefin, alkyne, aromatic and carbonyl carbons.

**Mass spectrometry:** Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic abundance and HRMS. Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, ortho effect.

Structure determination involving individual or combined use of the above spectral techniques.

[Reference Books: 13-18]

#### References:

1. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A, page no. 713-769, and B, Plenum Press.
3. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
4. Organic Chemistry, R.T. Morrison, R.N. Boyd and S.K. Bhattacharjee, Pearson Publication (7<sup>th</sup> Edition)
5. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
6. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
7. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
8. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
9. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.
10. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
11. Mechanism in Organic Chemistry, Peter Sykes, 6th  
Molecular Orbital and Organic chemical reactions, Ian Fleming Reference Edition, Wiley
12. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.
13. Spectrometric Identification of Organic Compounds, R. Silverstein, G.C Bassler and T.C. Morrill, John Wiley and Sons.
14. Organic Spectroscopy, William Kemp, W.H. Freeman & Company.
15. Organic Spectroscopy-Principles and Applications, Jagmohan, Narosa Publication.
16. Organic Spectroscopy, V.R. Dani, Tata McGraw Hill Publishing Co.

17. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Ltd.
18. Organic Reaction Mechanisms, V.K. Ahluwalia, R.K. Parasher, Alpha Science International, 2011.
19. Reactions, Rearrangements and Reagents by S. N. Sanyal
20. Name Reactions, Jie Jack Li, Springer
21. Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, M.G. Eller, and F.G. Favaloro, John Wiley & Sons.

**Organic Chemistry Practical  
Paper III**

**Course Code: PSCHP 203**

**Separation of Binary mixture using micro-scale technique**

1. Separation of binary mixture using physical and chemical methods.
2. Characterization of one of the components with the help of chemical analysis and confirmation of the structure with the help of derivative preparation and its physical constant.
3. Purification and determination of mass and physical constant of the second component.

The following types are expected:

- (i) Water soluble/water insoluble solid and water insoluble solid,
- (ii) Non-volatile liquid-Non-volatile liquid (chemical separation)
- (iii) Water-insoluble solid-Non-volatile liquid.

**Minimum three mixtures from each type and a total of ten mixtures are expected.**

**Reference:**

1. Systematic Qualitative organic analysis, H. Middleton (Orient Longman)
2. A Handbook of Organic Analysis, H.T. Clark (Orient Longman)
3. Systematic Identification of organic compounds, R.L. Shriner (John Wiley, New York)
4. Practical Organic Chemistry by Mann and Saunders.
5. Advance Practical Organic Chemistry, N.K. Vishnoi, Vikas Publication

**Paper IV**

**Analytical Chemistry: Course Code: PSCH 104 [60 L]**

**Unit I**

## **Chromatography [15 L]**

**Recapitulation of basic concepts in chromatography:** Classification of chromatographic methods, requirements of an ideal detector, types of detectors in LC and GC, comparative account of detectors with reference to their applications (LC and GC respectively), qualitative and quantitative analysis. [2 L]

Concept of plate and rate theories in chromatography: efficiency, resolution, selectivity and separation capability. Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions. [5 L]

**Gas Chromatography:** Instrumentation of GC with special reference to sample injection systems – split/splitless, column types, solid/ liquid stationary phases, column switching techniques, temperature programming, Thermionic and mass spectrometric detector, Applications. [3 L]

**High Performance Liquid Chromatography (HPLC):** Normal phase and reversed phase with special reference to types of commercially available columns (Use of C8 and C18 columns). Diode array type and fluorescence detector, Applications of HPLC. Chiral and ion chromatography. [5 L]

## **Unit II**

**X-ray spectroscopy:** principle, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy. [4 L]

**Mass spectrometry:** recapitulation, instrumentation, ion sources for molecular studies, electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources. Mass analyzers: Quadrupole, time of flight and ion trap. Applications. [6 L]

**Radioanalytical Methods** – recapitulation, isotope dilution method, introduction, principle, single dilution method, double dilution method and applications. [5 L]

## **Unit III**

### **Surface Analytical Techniques – [9 L]**

Introduction, Principle, Instrumentation and Applications of:

Scanning Electron Microscopy (SEM)

Scanning Tunneling Microscopy (STM)

Transmission Electron Microscopy (TEM)

Electron Spectroscopy (ESCA and Auger)

## **Unit IV**

### **Atomic Spectroscopy [6 L]**

Advantages and Limitations of AAS

Atomic Spectroscopy based on plasma sources – Introduction,  
Principle, Instrumentation and Applications.

**Electroanalytical Methods (Numericals are Expected)**

**Ion selective potentiometry and Polarography: [10 L]**

Ion selective electrodes and their applications (solid state, precipitate, liquid – liquid, enzyme and gas sensing electrodes), ion selective field effect transistors, biocatalytic membrane electrodes and enzyme based biosensors.

**Polarography:** Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves.

**Electrogravimetry:** Introduction, principle, instrumentation, factors affecting the nature of the deposit, applications. [3 L]

**Coulometry:** Introduction, principle, instrumentation, coulometry at controlled potential and controlled current [2 L]

#### References:

##### Unit I

1. Instrumental Analysis, Skoog, Holler & Crouch
2. HPLC Practical and Industrial Applications, 2<sup>nd</sup> Ed., Joel K. Swadesh, CRC Press

##### Unit II

1. Essentials of Nuclear Chemistry, H J Arnikar, New Age Publishers (2005)
2. Fundamentals of Radiochemistry D. D. Sood , A. V. R. Reddy and N. Ramamoorthy
3. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5<sup>th</sup> Edition, Ch: 12
4. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5<sup>th</sup> Edition, Ch: 20

##### Unit III

1. Instrumental Analysis by Douglas A. Skoog - F. James Holler - Crouch, Publisher: Cengage; Edition, (2003), ISBN-10: 8131505421, ISBN-13: 978-8131505427
2. Physical Principles of Electron Microscopy, An Introduction to TEM, SEM, and AEM
3. Authors: Ray F. Egerton, ISBN: 978-0- 387-25800- 3 (Print) 978-0- 387-26016- 7 (Online)
4. Modern techniques of surface science by D.P. Woodruff, T.A. Delchar, Cambridge Univ. Press, 1994.
5. Introduction to Scanning Tunneling Microscopy by C. J. Chen, Oxford University Press, New York, 1993.

6. 5. Transmission Electron Microscopy: A text book for Material Science, David B Williams and C., Barry Carter, Springer
7. Modern Spectroscopy, by J.M. Hollas, 3rd Edition (1996), John Wiley, New York
8. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
9. Instrumental Analysis by Douglas A. Skoog - F. James Holler - Crouch, Publisher: Cengage; Edition (2003), ISBN10: 8131505421, ISBN-13: 978-8131505427

#### Unit IV

1. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5<sup>th</sup> Edition, Harcourt College Publishers, 1998. Chapters - 23, 24, 25.
2. Analytical Chemistry Principles – John H Kennedy, 2nd edition, Saunders College Publishing (1990).
3. Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).
4. Vogel's Text book of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).
5. Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).
6. Instrumental Methods of Analysis Willard, Merrit, Dean and Settle, 7th edition, CBS publishers.

#### Analytical Chemistry Practical

##### Paper IV

##### Course Code: PSCHP 204

1. To determine percentage purity of sodium carbonate in washing soda pH metrically.
2. To determine amount of Ti(III) and Fe(II) in a mixture by titration with Ce(IV) potentiometrically.
3. To determine the percentage purity of a sample (glycine/sodium benzoate/primary amine) by titration with perchloric acid in a non aqueous medium using glass calomel system potentiometrically.
4. To determine the amount of nitrite present in the given water sample colorimetrically.
5. To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.
6. Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically.
7. To determine the percentage composition of HCl and H<sub>2</sub>SO<sub>4</sub> on weight basis in a

mixture of two by conductometric titration with NaOH and BaCl<sub>2</sub>.

8. To determine amount of potassium in the given sample of fertilizers using flame photometer by standard addition method.

#### References

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogel, 3<sup>rd</sup> Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas, Pearson education
3. Standard methods of chemical analysis, F. J. Welcher
4. Standard Instrumental methods of Chemical Analysis, F. J. Welcher
5. W.W.Scott."Standard methods of Chemical Analysis",Vol.I, Van Nostrand Company, Inc.,1939.
6. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals",Part- II, 4th Ed.,A Wiley Interscience Publication,New York,1978

## Practical Examination

Practical examination of each paper for 50 marks will be held for three and half hours  
Practical 40M  
Journal 5M  
Viva-voce 5M  
Total  
50M

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