

**Rayat Shikshan Sanstha's**  
**Karmaveer Bhaurao Patil College Vashi, Navi Mumbai**  
**Autonomous College**  
**[University of Mumbai]**  
**Syllabus for Approval**

**M.Sc.-I in Chemistry**

<b>Sr. No.</b>	<b>Heading</b>	<b>Particulars</b>
1	Title of Course	M.Sc.-I Chemistry
2	Eligibility for Admission	The B.Sc. degree examination of this university with chemistry 6 units or 3 units or degree of any other university recognized as equivalent
3	Passing Marks	Minimum 'D' Grade or equivalent minimum marks for passing at the Graduation level.
4	Ordinances/Regulations (if any)	
5	No. of Years/Semesters	One year/Two semester
6	Level	P.G. part-I
7	Pattern	Semester
8	Status	Revised
9	To be implemented from Academic year	2019-2020

AC – 02/03/2019

Item No: 2.8



**Rayat Shikshan Sanstha's  
KARMAVEER BHURAO PATIL COLLEGE, VASHI.  
NAVI MUMBAI**

**(AUTONOMOUS COLLEGE)**

Sector-15- A, Vashi, Navi Mumbai - 400 703

**Syllabus for M.Sc.-I in Chemistry**

**Program: M.Sc.**

**Course: M.Sc.-I Chemistry**

**(Choice Based Credit, Grading and Semester System  
with effect from the academic year 2018-2019)**

## **Preamble:**

The purpose of post-graduate education in Science is to create highly skilled man power in specific areas, which will lead to generation of new knowledge and creation of wealth for the country. Chemistry is a fundamental science and has contributed immensely to the improvement of the life of human beings by providing many of human requirements and essentialities. It is seen that developments in chemistry are crossing the traditional boundaries of scientific disciplines; the more inclination is seen towards biological sciences. New branches of chemistry are emerging and gaining importance, such as bioorganic chemistry, materials chemistry, computational chemistry etc. The practice of Chemistry at industrial scale also is undergoing radical changes and is based on deep understanding the chemical phenomena. The aid of computers has not only accelerated growth in the practice of Chemistry, but revolutionized the entire field.

A Chemist cannot isolate himself from other disciplines. Thus, after a long span of more and more specialization in graduate and post-graduate syllabi, a symbiotic interdisciplinary approach now seems to be more relevant. The practice of Chemistry, as is witnessed, over a span of more than a century has also created concomitant and perhaps unavoidable impacts of human environment. Though not a separate branch of Chemistry, Green Chemistry has emerged as a new approach to the practice of Chemistry on the background of sustainability. The Chemical industries now a days tries to develop eco-friendly processes and products which will reduce waste and prevent toxic substances from entering the environment. The principles and applications of Chemistry should be learnt on this background.

Thus this offers new chemical frontiers and tells us what benefits of taking up chemistry as a career. Chemists design reactions that will convert chemical substances around us into chemical substances that serve our needs today. Chemistry has become a crucial factor in the nation's economic well-being. The present Master's course is designed with an aim to prepare post graduates with the skills to solve problems requiring the application of chemical principles from each sub disciplines- organic, inorganic, physical, analytical chemistry. The Masters will have working knowledge of chemical instruments and laboratory techniques and be able to use those to design and carryout own research work or at industry level.

## Syllabus for M.Sc-I Chemistry

### Objectives of the Course:

1. To abreast the students about the current status and new developments in Chemistry.
2. To make the students aware of the impact of Chemistry on environment and imbibe the concept of sustainable developments
3. To educate the students with respect to skills and knowledge to practice chemistry in ways that are benign to health and environment.
4. To provide flexibility in selecting some of the courses as per the interest.
5. To make the students aware of resources and make them capable of mining the data.
6. To acquaint students with the specific areas of Organic, Inorganic & Analytical Chemistry
7. To develop analytical skills and critical thinking through application of theory knowledge into practical course
8. To enable students to understand chemistry and its industrial and social context

### Program Specific Outcomes:

1. The Students will learn various concepts of Core Inorganic Chemistry, organic, physical, analytical chemistry, their biological aspects and their application in day-to-day life.
2. They will be Competent to take challenging positions in industry, academics and government sectors by learning various analytical techniques such as UV, Raman, Mossbauer, XRD, XPS, AES, IR, NMR etc. and their applications.
3. They will be able to execute new ideas in the field of research and development using principles and techniques of science learned through seminars and the dissertation.
4. The students will improve their competencies on par with their counterparts in premier institutions across the nation.
5. The students will become technically sound to handle the advance instruments.
6. The students will intensify their desire to contribute to the nation in the capacity of chemist or as innovator by taking up research career afterwards.
7. The students will become well versed in the mechanisms of all types of high level and complicated chemical reactions.
8. The students thereby will contribute learned knowledge for betterment of oneself, society and nation.
9. Students will appreciate the central role of chemistry in our society and use this as a basis for ethical behavior in issues facing chemists including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health, and medicine.

## Course Outcomes

Course Code	Title of Course	Unit	Course Outcome
			After successful completion of each course in Chemistry a learner should be able to;
PGCH101	Physical Chemistry	Unit-I Thermodynamics - I	<ol style="list-style-type: none"> <li>To discuss state functions and exact differentials.<sup>[2]</sup></li> <li>To deduce Maxwell equations and its thermodynamic relations.<sup>[3]</sup></li> <li>To describe Joule Thomson experiment and related terms.<sup>[2]</sup></li> <li>To apply third law of thermodynamics for finding entropy change in phase transition.<sup>[3]</sup></li> <li>To explain absolute entropies, standard molar entropies and residual entropy.<sup>[2]</sup></li> </ol>
		Unit II Quantum Chemistry	<ol style="list-style-type: none"> <li>To compare classical mechanics with quantum mechanics.<sup>[4]</sup></li> <li>To outline Schrodinger wave equation, properties of wave function and its properties.<sup>[3]</sup></li> <li>To explain operators and their algebra.<sup>[2]</sup></li> <li>To apply quantum mechanics to free particle, particle in one-, two- and three-dimensional box.<sup>[3]</sup></li> <li>To discuss concept of quantization, quantum numbers and degeneracy of energy level.<sup>[2]</sup></li> </ol>
		Unit III Chemical Dynamics I	<ol style="list-style-type: none"> <li>To recite rate laws, differential rate equations, consecutive reactions.<sup>[2]</sup></li> <li>To discuss the kinetics and mechanism of chain reaction, inorganic and organic decomposition reactions.<sup>[2]</sup></li> <li>To describe Gas phase explosion reaction between H<sub>2</sub> and O<sub>2</sub>.<sup>[2]</sup></li> <li>To illustrate kinetics and mechanism of stepwise and chain polymerization reaction.<sup>[2]</sup></li> <li>To explain Lindeman-Hinshelwood, RRK and RRKM theory for unimolecular reactions.<sup>[2]</sup></li> </ol>
		Unit-IV Electrochemistry	<ol style="list-style-type: none"> <li>To deduce Debye-Huckel limiting law on the basis of Debye-Huckel theory.<sup>[3]</sup></li> <li>To solve numerical problems on Debye-Huckel limiting law.<sup>[3]</sup></li> <li>To explain Debye-Huckel-Onsager equation, its validity and deviations.<sup>[2]</sup></li> <li>To describe alkaline fuel cells, phosphoric acid fuel cells and high temperature fuel cell.<sup>[2]</sup></li> <li>To describe acid, alkaline, rechargeable battery, Li ion battery.<sup>[2]</sup></li> </ol>
		Unit I Chemical	<ol style="list-style-type: none"> <li>Derive wave functions for <math>sp</math>, <math>sp^2</math>, <math>sp^3</math> orbital hybridization types considering only sigma</li> </ol>

PGCH102	Inorganic Chemistry	Bonding	<p>bonding. <sup>[3]</sup></p> <ol style="list-style-type: none"> <li>2. Demonstrate Molecular Orbital Theory for Polyatomic species for various species and draw energy level diagrams. <sup>[2]</sup></li> <li>3. Summarize Van der Waal's forces, ion-dipole, dipole-dipole, London forces. <sup>[2]</sup></li> </ol>
		Unit-II Molecular Symmetry and Group Theory	<ol style="list-style-type: none"> <li>1. To recite concept of symmetry elements in molecules. <sup>[2]</sup></li> <li>2. Illustrate dipole moment and bond order of the various inorganic molecule by applying symmetry rules. <sup>[2]</sup></li> <li>3. To evaluate relations between Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. <sup>[2]</sup></li> <li>4. To construct character tables for point groups <math>C_{2v}</math>, <math>C_{3v}</math> and <math>D_{2h}</math> <sup>[2]</sup></li> <li>5. To apply group theory on molecules to find out Symmetry adapted linear combinations. <sup>[3]</sup></li> </ol>
		Unit-III Materials Chemistry and Nano materials	<ol style="list-style-type: none"> <li>1. To explain electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones. <sup>[2]</sup></li> <li>2. To illustrate different methods of preparation for inorganic solids and nanomaterials. <sup>[2]</sup></li> <li>3. Categorize different applications of nanomaterials according to their use. <sup>[2]</sup></li> </ol>
		Unit - IV Characterization of Coordination compounds	<ol style="list-style-type: none"> <li>1. To illustrate effect of ligand field on energy levels of transition metal ions. <sup>[2]</sup></li> <li>2. To derive free ion Terms, Spin Orbit coupling, R-S terms <sup>[3]</sup></li> <li>3. To calculate electronic parameters for electronic states of metal ions <sup>[3]</sup></li> <li>4. To determine formation constants of metal complexes. <sup>[2]</sup></li> </ol>
PGCH103	Organic Chemistry	Physical Organic Chemistry	<ol style="list-style-type: none"> <li>1. To understand the thermodynamic and kinetic requirements of a reaction<sup>[2]</sup></li> <li>2. To know Curtin-Hammett Principle<sup>[2]</sup></li> <li>3. To know Methods for determining mechanism of a reaction<sup>[2]</sup></li> <li>4. To understand Kinetic vs thermodynamic control of organic reactions<sup>[2]</sup></li> <li>5. To understand Product analysis, kinetic studies<sup>[2]</sup></li> <li>6. To know Factors affecting acidity and basicity<sup>[2]</sup></li> <li>7. To exemplify the acid base properties <sup>[2]</sup></li> <li>8. To Study Acids and Bases approaches and their applications. <sup>[2]</sup></li> </ol>
		Nucleophilic substitution reactions and Aromaticity	<ol style="list-style-type: none"> <li>1. To understand the various aliphatic and Aromatic nucleophilic substitution reactions mechanism and factors affecting them <sup>[2]</sup></li> <li>2. To understand SN1, SN2, SN<sup>1</sup> reactions, mixed SN1 and SN2 reactions in details <sup>[2]</sup></li> <li>3. To understand Ambident nucleophiles. <sup>[2]</sup></li> <li>4. To know the Structural, thermochemical, and magnetic criteria for aromaticity</li> <li>5. To remember the Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral</li> </ol>

			<p>center<sup>[2]</sup></p> <ol style="list-style-type: none"> <li>To study the various basic concept of Aromaticity<sup>[2]</sup></li> <li>To know Homoaromatic compounds. <sup>[2]</sup></li> </ol>
		Stereochemistry	<ol style="list-style-type: none"> <li>To know Principles of axial and planar chirality<sup>[2]</sup></li> <li>To understand the basic concept and applications of the stereochemistry. <sup>[2]</sup></li> <li>To study the various oxidation and reduction reagents and their applications <sup>[2]</sup></li> <li>To remember Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature<sup>[2]</sup></li> <li>To know the basic concept of 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. <sup>[2]</sup></li> <li>To know the Chiral and prochiral centres; prochiral axis and prochiral plane<sup>[2]</sup></li> </ol>
		Oxidation and Reduction	<ol style="list-style-type: none"> <li>To know Oxidation: General mechanism, selectivity, and important applications of the<sup>[2]</sup></li> <li>To know the the various oxidizing agent Chromium reagents such as K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>/H<sub>2</sub>SO<sub>4</sub> (Jones reagent), CrO<sub>3</sub>-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. <sup>[2]</sup></li> <li>To study Oxidation involving C-C bonds cleavage<sup>[2]</sup></li> <li>To know Oxidation of aldehydes and ketones<sup>[2]</sup></li> <li>To know Reduction: General mechanism, selectivity, and important applications of the following reducing reagents: <sup>[2]</sup></li> <li>To study Reduction of CO to CH<sub>2</sub> in aldehydes and ketones<sup>[2]</sup></li> <li>To know Dissolving metal reductions <sup>[2]</sup></li> </ol>
PGCH104	Analytical Chemistry	Language of Analytical Chemistry	<ol style="list-style-type: none"> <li>To aware about the applicability of analytical chemistry in various fields <sup>[2]</sup></li> <li>To remember Analytical perspective, Common analytical problems, terms involved in analytical chemistry<sup>[2]</sup></li> <li>To introduce research attitude in learners<sup>[2]</sup></li> <li>To remember and an overview of analytical methods<sup>[2]</sup></li> <li>To evaluate problems related to chemical analysis and interpret analytical results</li> <li>To understand the terms involved in analytical chemistry and statistical calculations of observed</li> </ol>

			<p>data <sup>[2]</sup></p> <ol style="list-style-type: none"> <li>To Know Basic concepts of Safety in Laboratories, <sup>[2]</sup></li> <li>To study GLP<sup>[2]</sup></li> <li>To Understand Quality Management System (QMS) <sup>[2]</sup></li> </ol>
		Quality in Analytical Chemistry	<ol style="list-style-type: none"> <li>To study Concentration of a solution based on volume and mass units. <sup>[2]</sup></li> <li>To solve Problems based on Calculations of ppm, ppb and dilution of the solutions, concept of mmol <sup>[2]</sup></li> <li>To know Concept of formation constants, stability and instability constants, stepwise formation constants. <sup>[2]</sup></li> <li>To remember chemical calculations in analytical chemistry <sup>[2]</sup></li> </ol>
		Molecular Ultraviolet and Visible Spectroscopy	<ol style="list-style-type: none"> <li>To remember basic concepts, Electromagnetic spectrum, Sources, Detectors, sample containers. <sup>[2]</sup></li> <li>To Know Molecular Ultraviolet and Visible Spectroscopy <sup>[2]</sup></li> <li>To Study Infrared Absorption Spectroscopy <sup>[2]</sup></li> <li>To Introduced basic principles of diffuse reflectance spectroscopy <sup>[2]</sup></li> <li>To Know the concept of spectroscopy with theoretical and practical aspects <sup>[2]</sup></li> </ol>
		Thermal Methods	<ol style="list-style-type: none"> <li>To remember introduce basic knowledge of various thermal methods used in characterization. <sup>[2]</sup></li> <li>To remember of types of thermal methods, comparison between TGA and DTA. <sup>[2]</sup></li> <li>To know Differential Scanning Calorimetry. <sup>[2]</sup></li> <li>To Apply - Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage crystallinity, oxidative stability in various Material <sup>[3]</sup></li> </ol>
PGCHP101	Physical Chemistry Practical		<ol style="list-style-type: none"> <li>To understand how to determine the heat of solution at different temperature. <sup>[2]</sup></li> <li>To study ionic strength of various inorganic salts. <sup>[2]</sup></li> <li>To evaluate kinetics of the reactions. <sup>[4]</sup></li> <li>To understand various methods of graph plotting. <sup>[2]</sup></li> <li>To understands various instrumental techniques. <sup>[2]</sup></li> </ol>
PGCHP102	Inorganic Chemistry Practical		<ol style="list-style-type: none"> <li>To prepare various inorganic complexes and their characterizations. <sup>[2]</sup></li> <li>To determine the electrolytic nature of inorganic compounds. <sup>[2]</sup></li> <li>Determination of equilibrium constants of inorganic compounds. <sup>[2]</sup></li> </ol>
PGCHP103	Organic Chemistry Practical	1.	<ol style="list-style-type: none"> <li>Planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS should be learnt. <sup>[6]</sup></li> </ol>



			<p>3. Purify the product by crystallization. Formation and purity of the product should be checked by TLC <sup>[2]</sup></p> <p>4. Report yield and melting point of the purified product. <sup>[2]</sup></p>
PGCHP104	Analytical Chemistry Practical	1.	<p>2. Determination of assay of compounds. <sup>[2]</sup></p> <p>3. To understand spectrophotometric analysis of the various organic and inorganic compounds. <sup>[2]</sup></p> <p>4. To study the ion exchange capacity and its applications. <sup>[2]</sup></p> <p>5. Determination of nitro compounds use volumetric method <sup>[2]</sup></p>

**\*Note: [1]: Remembering, [2]: Understanding, [3]: Applying, [4]: Analysing, [5]: Evaluating, [6]: Creating**

## Scheme of examination for Each Semester:

**Continuous Internal Evaluation: 40 Marks** (Common Written Test-20 Marks & 20 Marks for- Seminar/Assignment, Projects, Group discussion, Open book test, online test etc.)

**Semester End Examination: 60 Marks will be as follows:**

<b>I.</b>	<b>Theory:</b> The Semester End Examination for theory course work will be conducted as per the following scheme.	
	Each theory paper shall be of two and half hour duration.	
	All questions are compulsory and will have internal options.	
	Q – I	From Unit – I (having internal options.) 12 M
	Q – II	From Unit – II (having internal options.) 12 M
	Q – III	From Unit – III (having internal options.) 12 M
	Q – IV	From Unit – III (having internal options.) 12 M
Q – V	Questions from all the FOUR Units with equal weightage of marks allotted to each Unit. 12 M	
<b>II.</b>	<b>Practical</b>	The Semester End Examination for practical course work will be conducted as per the following scheme.
<b>Sr. No.</b>	<b>Particulars of Semester End Practical Examination</b>	<b>Marks%</b>
1	Laboratory Work	80
2	Journal	10
3	Viva	10
	<b>TOTAL</b>	<b>100</b>

**Choice Based Credit, Grading and Semester System with effect from the  
academic year 2018-2019**

**M.Sc.-I Chemistry**

**Semester - I**

Course Code	Unit	Topics	Credits	L/Week
PGCH101	I	Thermodynamics-I	4	1
	II	Quantum Chemistry		1
	III	Chemical Dynamics-I		1
	IV	Electrochemistry		1
PGCH102	I	Chemical Bonding	4	1
	II	Molecular Symmetry and Group Theory		1
	III	Materials Chemistry and Nano materials		1
	IV	Characterization of Coordination compounds		1
PGCH103	I	Physical Organic Chemistry	4	1
	II	Nucleophilic substitution reactions and Aromaticity		1
	III	Stereochemistry		1
	IV	Oxidation and Reduction		1
PGCH104	I	Language of Analytical Chemistry	4	1
	II	Quality in Analytical Chemistry		1
	III	Molecular Ultraviolet and Visible Spectroscopy		1
	IV	Thermal Methods		1
PGCHP101 PGCHP102 PGCHP103 PGCHP104	-	Practical Course	8	16

**Note:** 1. Blue Highlighted Topic / Course has focus on employability/ entrepreneurship/skill development  
2. Green Highlighted Topic / Course is related to local/national/regional & global development needs.

**Semester – I**  
**Paper I**

**Physical Chemistry:**  
**Course Code: PGCH 101**

**[60 L]**

**Unit - I**

**Thermodynamics-I [15]**

- 1.1. State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; its significance and applications to ideal gases, Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of van der Waals constants. **[8L]**
- 1.2. Third law of Thermodynamics, Entropy change for a phase transition, absolute entropies, determination of absolute entropies in terms of heat capacity, standard molar entropies and their dependence on molecular mass and molecular structure, residual entropy. **[7L]**

**Unit II**

**Quantum Chemistry: [15L]**

- 2.1. Classical Mechanics, failure of classical mechanics: Need for Quantum Mechanics.
- 2.2. Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions.
- 2.3. Operators and their algebra, linear operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, Eigen functions, Eigen values and Eigen value equation, Schrödinger wave equation as the Eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, Postulates of Quantum Mechanics, Schrodinger's Time independent wave equation from Schrodinger's time dependent wave equation.
- 2.4. Application of quantum mechanics to the following systems:
  - a) Free particle, wave function and energy of a free particle.
  - 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.

**Unit III**

**Chemical Dynamics-I [15L]**

3.1. 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.

3.2. 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.

3.3. Reaction in Gas Phase

Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kassel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.

## Unit IV

### Electrochemistry [15L]

#### Recapitulation – basics of electrochemistry.

- 4.1. Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and its extension to higher concentration (derivations are expected).
- 4.2. 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.
- 4.3. Electrochemical storage Devices: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]
- 4.4. Batteries: Introduction to Battery, acid, alkaline, rechargeable battery, Li ion battery, Li ion polymer battery, Design and terminology, Applications

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

#### 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. 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*

## Paper I

### Physical Chemistry Practical

Course Code: PGCHP 101

(60L)

#### Learning objectives:

6. To understand how to determine the heat of solution at different temperature.
7. To study ionic strength of various inorganic salts.
8. To evaluate kinetics of the reactions.
9. To understand various methods of graph plottings.
10. To understands various instrumental techniques.

#### 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 weakmono-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.

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## Paper II

**Inorganic Chemistry:**  
**Course Code: PGCH 102**

**(60 L)**

### Unit I

#### Chemical Bonding: [15 L]

- 1.1 **Recapitulation of hybridization** Derivation of wave functions for  $sp$ ,  $sp^2$ ,  $sp^3$  orbital hybridization types considering only sigma bonding.
- 1.2 Discussion of involvement of  $d$  orbitals in various types of hybridizations. Formal charge with examples.
- 1.3 Critical analysis of VBT.
- 1.4 Molecular Orbital Theory for diatomic species of First transition Series.
- 1.5 Molecular Orbital Theory for Polyatomic species considering  $\sigma$  bonding for  $S_6$ ,  $CO_2$ ,  $B_2H_6$ ,  $I_3^-$  molecular species.
- 1.6 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]

- 2.1. Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules.
- 2.2. Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups.
- 2.3. 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.
- 2.4. Applications of Group Theory
  - (a) Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in  $AB_n$  ( $H_2O$ ,  $NO_2$ ,  $CH_4$ ) molecule.
  - (b) Mulliken's notations for irreducible representations.
  - (c) Reduction of reducible representations using reduction formula.
  - (d) Group-subgroup relationships.



## Unit–III

### Materials Chemistry and Nano materials: [15 L]

#### 3.1 Solid State Chemistry

- 3.1.1. Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.
- 3.1.2. 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>)].
- 3.1.3. 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)

#### 3.2 Nanomaterials

- 3.2.1. Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation.
- 3.2.2. Applications in the field of semiconductors, solar cells

## Unit - IV

### Characterization of Coordination compounds [15L]

- 4.1 Ligand field theory of co-ordination complexes: Effect of ligand field on energy levels of transition metal ions, Free ion Terms, Spin Orbit coupling, R-S terms
- 4.2. Spectral calculations using Orgel and Tanabe-Sugano diagram, calculation of electronic parameters such as  $\Delta$ , B, C, Nephelauxetic effect, Nephelauxetic ratio.
- 4.3. 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.
6. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.
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.

## Paper II

### Inorganic Chemistry Practical

Course Code: PGCHP 102

(60L)

#### Inorganic Preparations (Synthesis and Characterization)

1. Synthesis of chloropentaammine cobalt (III) chloride
2. Synthesis of nitropentaammine cobalt (III) chloride
3. Synthesis of nitritopentaammine cobalt (III) chloride
4. Tetrammine monocarbonato Cobalt (III) Nitrate  $[\text{Co}(\text{NH}_3)_4\text{CO}_3]\text{NO}_3$
5. Bis (ethylenediammine) Copper (II) Sulphate  $[\text{Cu}(\text{en})_2]\text{SO}_4$
6. Hydronium dichloro bis ( dimethylglyoximato) Cobaltate(III)  $\text{H}[\text{Co}(\text{dmgH})_2\text{Cl}_2]$
7. Bis-(tetraethylammonium) tetrachloro Cuprate (II)  $(\text{Et}_4\text{N})_2[\text{CuCl}_4]$
8. Bis-(tetraethylammonium) tetrachloro Nickelate (II)  $(\text{Et}_4\text{N})_2[\text{NiCl}_4]$
9. Bis-(tetraethylammonium) tetrachloro Cobaltate (II)  $(\text{Et}_4\text{N})_2[\text{CoCl}_4]$

#### Instrumentation

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

#### References:

1. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
2. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By: Dr Deepak Pant

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## Paper III

**Organic Chemistry:**  
**Course Code: PGCH 103**

**(60 L)**

### Unit I

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

- 1.1. 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.
- 1.2. 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.
- 1.3. Acids and Bases:** Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity. Comparative study of acidity and basicity of organic compounds on the basis of pK<sub>a</sub> values, Acid and base catalysis – general and specific catalysis with examples.

### Unit II

#### Nucleophilic substitution reactions and Aromaticity

##### 2.1. Nucleophilic substitution reactions: (9 L)

**2.1.1. 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 π-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' and S<sub>N</sub>2' reactions. S<sub>N</sub> at sp<sup>2</sup> (vinylic) carbon.

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

##### 2.2. Aromaticity: (6 L)

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

**2.2.2.** 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<sub>60</sub>).

## Unit-III

### Stereochemistry: (15 L)

- 3.1. Molecules with tri- and tetra-coordinate centers:** Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities.
- 3.2. 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 pseudo asymmetric centers. R-S nomenclature for chiral centers in acyclic and cyclic compounds.
- 3.3. 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.
- 3.4. 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 centers ii) a chiral as well as a prochiral center, a prochiral axis iv) a prochiral plane v) pro-pseudoasymmetric center. Symbols for enantiotopic and diastereotopic faces.

## Unit-IV

### Oxidation and Reduction: (15 L)

- 4.1. Oxidation:** General mechanism, selectivity, and important applications of the followings:
- 4.1.1. Dehydrogenation:** Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).
- 4.1.2. 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.

**4.1.3. Oxidation involving C-C bonds cleavage:** Glycols using  $\text{HIO}_4$ ; carbon-carbon double bond using ozone,  $\text{KMnO}_4$ ,  $\text{CrO}_3$ ,  $\text{NaIO}_4$  and  $\text{OsO}_4$ ; aromatic rings using  $\text{NaIO}_4$ .

**4.1.4. Oxidation involving replacement of hydrogen by oxygen:** oxidation of  $\text{CH}_2$  to  $\text{CO}$  by  $\text{SeO}_2$ ,

**4.1.5. Oxidation of aldehydes and ketones:** with  $\text{H}_2\text{O}_2$  (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)

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

**4.2.1. Reduction of  $\text{CO}$  to  $\text{CH}_2$  in aldehydes and ketones-** Clemmensen reduction, Wolff-Kishner reduction.

**4.2.2. Metal hydride reduction:** Boron reagents ( $\text{NaBH}_4$ ,  $\text{NaCNBH}_3$ , diborane, 9-BBN,  $\text{Na}(\text{OAc})_3\text{BH}$ ,  $\cdot\text{NH}_2\text{NH}_2$  (diimide reduction)).MPV Reduction,

**4.2.4. Dissolving metal reductions:**  $\text{Li}/\text{Na}$ -liquid  $\text{NH}_3$  mediated reduction (Birch reduction) of aromatic compounds and acetylenes.

#### 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.

## Organic Chemistry Practical

Course Code: PGCHP 103

(60 L)

### One step preparations (1.0 g scale) (Any Ten)

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
11. Radical coupling reaction (Preparation of 1,1-bis-2-naphthol)
12. Pechmann condensation for coumarin synthesis (Clay catalyzed solid state synthesis of 7-hydroxy-4-methylcoumarin)

### 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

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## Paper IV

**Analytical Chemistry:**  
**Course Code: PGCH 104**

**(60 L)**

### Unit - I

#### **1.1 Language of Analytical Chemistry [8 L]**

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

**1.1.2** 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.

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

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

#### **1.2 Quality in Analytical Chemistry: [7 L]**

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

Evolution and significance of Quality Management, types of quality standards for laboratories, total quality management (TQM), quality audits and quality reviews, responsibility of laboratory staff for quality and problems.

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

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

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

Principle, Objective, OECD guidelines

### 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.
- Stoichiometry of chemical reactions, concept of kg mol, limiting reactant, theoretical and practical yield.
- 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.

### **Unit III**

#### **Optical Methods [15 L]**

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

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

**3.1.2** Laser as a source of radiation, Fibre optics

**3.1.3** Introduction of Fourier Transform

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

Numericals are expected

**3.2.1** 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

**3.2.2** Dual spectrometry – Introduction, Principle, Instrumentation and Applications

##### **3.3 Infrared Absorption Spectroscopy [6 L]**

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

**3.3.2** FTIR and its advantages

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

**3.3.4** Introduction and basic principles of diffuse reflectance spectroscopy.

### **Unit - IV**

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

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

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

**4.1.3 Applications** - Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage crystallinity, oxidative stability.

### References

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, Parag Diwan, 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/rtp.1996.1076. PMID 9056496.

## Analytical Chemistry Practical

Course Code: PGCHP 104

(60L)

### Practical

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  $\text{TiCl}_3$ .
8. Determination of alcohol from given sample by Spectrophotometrically.

#### 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.

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**Choice Based Credit, Grading and Semester System with effect from the  
academic year 2018-2019**

**M.Sc.-I Chemistry**

**Semester - II**

<b>Course Code</b>	<b>Unit</b>	<b>Topics</b>	<b>Credits</b>	<b>L/Week</b>
PGCH201	I	Chemical Thermodynamics II	4	1
	II	Quantum Chemistry II		1
	III	Chemical Kinetics and Molecular Reaction Dynamics		1
	IV	Solid State Chemistry and Phase Equilibria		1
PGCH202	I	Inorganic Reaction Mechanism	4	1
	II	Organometallic Chemistry of Transition metals		1
	III	Environmental Chemistry		1
	IV	Bioinorganic Chemistry		1
PGCH203	I	Introduction to Molecular Orbital Theory for Organic Chemistry	4	1
	II	Reactions and Rearrangements		1
	III	Alkylation of Nucleophilic Carbon Intermediates		1
	IV	NMR spectroscopy and Mass spectrometry		1
PGCH204	I	Chromatography	4	1
	II	Analytical Spectroscopy		1
	III	Surface Analytical Techniques		1
	IV	Electroanalytical Methods		1
PGCHP201 PGCHP202 PGCHP203 PGCHP204	-	Practical Course	8	16
<p><b>Note:</b> 1. Blue Highlighted Topic / Course has focus on employability/ entrepreneurship/skill development 2. Yellow Highlighted Topic / Course is related to professional ethics, gender, human values, Environment &amp; sustainability</p>				

## Course Outcomes

Course Code	Title of Course	Unit	Course Outcome
			After successful completion of each course in Chemistry a learner should be able to;
PGCH201	Physical Chemistry	Unit-I Chemical Thermodynamics	<ol style="list-style-type: none"> <li>To describe the determination of fugacity of real gases using graphical method and equation of state. <sup>[2]</sup></li> <li>To describe Gibb's energy of mixing, entropy and enthalpy of mixing and to solve problems on it. <sup>[2]</sup></li> <li>To calculate partial molar volume and partial molar enthalpy. <sup>[3]</sup></li> <li>To deduce Laplace equation, Kelvin equation, Gibb's adsorption isotherm and BET isotherm. <sup>[3]</sup></li> <li>To explain the role of standard free energy in biochemical reactions. <sup>[2]</sup></li> </ol>
		Unit II Quantum Chemistry II	<ol style="list-style-type: none"> <li>To discuss Schrodinger wave equation, separation of variables, spherical harmonics for Rigid rotor. <sup>[2]</sup></li> <li>To discuss Schrodinger wave equation, separation of variables for Hydrogen. <sup>[2]</sup></li> <li>To construct probability density curves, radial and angular plots for different orbitals. <sup>[2]</sup></li> <li>To formulate the expressions for total wave functions for 1s, 2s, 2p and 2d orbitals. <sup>[3]</sup></li> <li>To apply Schrodinger equation to two electron system. <sup>[3]</sup></li> </ol>
		Unit III Chemical Kinetics and molecular Reaction Dynamics	<ol style="list-style-type: none"> <li>To discuss the influence of solvent Dielectric constant and ionic strength on reactions in solutions. <sup>[2]</sup></li> <li>To describe the kinetics of enzyme catalyzed reactions. <sup>[2]</sup></li> <li>To analyze Lineweaver-Burk and Eadie's plots. <sup>[3]</sup></li> <li>To discuss competitive, Non-competitive and Uncompetitive inhibition of enzyme action. <sup>[2]</sup></li> <li>To explain kinetics of reactions in solid state. <sup>[2]</sup></li> </ol>
		Unit IV Solid State Chemistry and phase equilibria	<ol style="list-style-type: none"> <li>To describe diagrammatically Zero, One- and Two-dimensional defects. <sup>[2]</sup></li> <li>To outline the terms involved in phase rule <sup>[2]</sup></li> <li>To formulate the phase rule. <sup>[3]</sup></li> <li>To construct phase diagrams for two component Solid-Gas and Solid-Liquid systems. <sup>[3]</sup></li> <li>To describe three component system containing one pair and two pair of partially miscible liquids. <sup>[2]</sup></li> </ol>
		Unit I Inorganic Reaction Mechanism	<ol style="list-style-type: none"> <li>To apply concept of Mechanism of trans-effect and write substitution reactions of square planar complex reactions. <sup>[3]</sup></li> <li>To demonstrate complimentary and non-complimentary reactions. <sup>[3]</sup></li> <li>To illustrate Isomerization and racemization in</li> </ol>

PGCH202	Inorganic Chemistry		Stereochemistry of substitution reactions of octahedral complexes. <sup>[3]</sup>
		Unit II Organometallic Chemistry of Transition metals	<ol style="list-style-type: none"> <li>1. To analyze stability of inorganic complexes based 18 &amp; 16 electron rule. <sup>[4]</sup></li> <li>2. To discuss preparation and properties of different inorganic compounds. <sup>[2]</sup></li> <li>3. To evaluate structure and bonding on the basis of VBT and MOT in organometallic compound <sup>[3]</sup></li> </ol>
		Unit III Environmental Chemistry	<ol style="list-style-type: none"> <li>1. To discuss toxicity of different metallic species. <sup>[2]</sup></li> <li>2. To write a report on toxic chemicals present in laboratory and its toxic effects. <sup>[6]</sup></li> <li>3. To summarize Sources and biological implication of radioactive materials <sup>[2]</sup></li> </ol>
		Unit IV Bioinorganic Chemistry	<ol style="list-style-type: none"> <li>1. To describe biological oxygen carriers present in different living species. <sup>[2]</sup></li> <li>2. To compare pH dependence of oxygen affinity in haemoglobin and myoglobin and its implications <sup>[3]</sup></li> <li>3. To paraphrase Copper containing enzymes, nitrogen fixation, metal ion transport and storage <sup>[2]</sup></li> <li>4. To summarize medicinal applications of inorganic compounds <sup>[2]</sup></li> <li>5. To describe mechanism for anti-cancer activity of cis-platin <sup>[2]</sup></li> </ol>
PGCH203	Organic Chemistry	Introduction to Molecular Orbital Theory for Organic Chemistry	<ol style="list-style-type: none"> <li>1) To understand the basic concept of Molecular Orbital Theory for Organic Chemistry and its applications <sup>[2]</sup></li> <li>2) To know Formation of <math>\sigma</math>- and <math>\pi</math>-MOs by using LCAO method<sup>[2]</sup></li> <li>3) To know HOMO and LUMO and significance of HOMO-LUMO<sup>[2]</sup></li> <li>4) To know the Application of FMO concepts in (a) <math>S_N^2</math> reaction, (b) Lewis acid base adducts (<math>BF_3-NH_3</math> complex), (c) ethylene dimerization to butadiene, (d) Diels-Alder cycloaddition, <sup>[2]</sup></li> <li>5) To know regioselective reaction of allyl cation with allyl anion (f) addition of hydride to formaldehyde. <sup>[2]</sup></li> <li>6) To study basic principal and applications of U.V.and I.R.Spectroscopy <sup>[2]</sup></li> <li>7) To understand the basic reaction mechanism with some named reactions and rearrangements <sup>[2]</sup></li> </ol>
		Reactions and Rearrangements	<ol style="list-style-type: none"> <li>1. To know Reactions: Baylis-Hilman reaction, McMurry Coupling, Nef reaction, Passerini reaction. <sup>[2]</sup></li> <li>2. To study concerted rearrangements: Hofmann, Curtius, Lossen, Schmidt, and Wolff. <sup>[2]</sup></li> <li>3. To know Cationic rearrangements: Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein. <sup>[2]</sup></li> <li>4. To know Anionic rearrangements: Brook, Neber, Von Richter, Wittig, Gabriel-Colman, <sup>[2]</sup></li> </ol>
		Alkylation of	<ol style="list-style-type: none"> <li>1. To understand carbanion approach with respect to Alkylation of Nucleophilic Carbon Intermediates<sup>[2]</sup></li> </ol>

		Nucleophilic Carbon Intermediates	<ol style="list-style-type: none"> <li>To study details in basic Reaction mechanism of carbon nucleophiles with carbonyl groups<sup>[2]</sup></li> <li>To know the Nitrogen analogs of enols and enolates-Enamines and Imines anions, alkylation of enamines and imines<sup>[2]</sup></li> <li>To remember the Addition reactions with amines and iminium ions; Mannich reaction<sup>[2]</sup></li> <li>To understand the basic principal and applications of NMR spectroscopy, <sup>13</sup>C NMR spectroscopy and Mass spectrometry<sup>[2]</sup></li> <li>To learn Structure determination involving individual or combined use of the above spectral techniques. <sup>[2]</sup></li> <li>To know Amine catalyzed condensation reaction: Knoevenagel reaction. <sup>[2]</sup></li> </ol>
		NMR spectroscopy and Mass spectrometry	<ol style="list-style-type: none"> <li>To know Proton magnetic resonance spectroscopy<sup>[2]</sup></li> <li>To know <sup>13</sup>C NMR spectroscopy: Theory and comparison with proton NMR<sup>[2]</sup></li> <li>To know Mass spectrometry in details <sup>[2]</sup></li> <li>To know and solve Structure determination involving individual or combined use of the above spectral techniques. <sup>[2]</sup></li> </ol>
PGCH204	Analytical Chemistry	Chromatography	<ol style="list-style-type: none"> <li>To Remember basic concepts in chromatography. <sup>[2]</sup></li> <li>To study Concept of plate and rate theories in chromatography. <sup>[2]</sup></li> <li>To know Gas Chromatography<sup>[2]</sup></li> <li>To study High Performance Liquid Chromatography (HPLC) <sup>[2]</sup></li> </ol>
		Analytical Spectroscopy	<ol style="list-style-type: none"> <li>To know X-ray spectroscopy, Mass spectrometry<sup>[2]</sup></li> <li>To know the various types of modern method of separation techniques used in various fields. <sup>[2]</sup></li> <li>To apply applicability of miscellaneous techniques in various fields. <sup>[3]</sup></li> </ol>
		Surface Analytical Techniques	<ol style="list-style-type: none"> <li>To study the different types of Surface Analytical Techniques. <sup>[2]</sup></li> <li>To apply the basic knowledge of atomic absorption spectroscopy and its applications. <sup>[3]</sup></li> </ol>
		Electroanalytical Methods	<ol style="list-style-type: none"> <li>To distinguish types of Electro analytical techniques used in quantitative and qualitative analysis. <sup>[3]</sup></li> <li>To Understand stake holders to various modern instrumental methods of analysis and separation techniques</li> <li>To know basic analytical techniques and practical aspects of classical chemical analysis. <sup>[2]</sup></li> <li>To apply a basic knowledge and understanding of core principals of analytical chemistry. <sup>[3]</sup></li> <li>To Know Coulometer <sup>[2]</sup></li> <li>To know Polarography: Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves. <sup>[2]</sup></li> </ol>
PGCHP201	Physical Chemistry		<ol style="list-style-type: none"> <li>To plot of various orbitals on graph paper. <sup>[3]</sup></li> <li>To observe kinetics of various reactions. <sup>[2]</sup></li> </ol>

	Practical		3) To apply concept of phase diagram. <sup>[3]</sup> 4) To know use of various instrument for analysis. <sup>[2]</sup>
PGCHP20 2	Inorganic Chemistry Practical		1. To analyse various ore and alloy for its. 2. To observe redox titrations <sup>[2]</sup> 3. To estimate amount of metal potentiometrically in given sample. <sup>[2]</sup>
PGCHP20 3	Organic Chemistry Practical		1. To enhance the separation techniques for organic compounds. <sup>[2]</sup> 2. To understand solubility of organic compound in different solvents. <sup>[2]</sup> 3. Determination of type and functional group of the organic compound <sup>[2]</sup>
PGCHP20 4	Analytical Chemistry Practical		1. To determine percentage purity of sodium carbonate in washing soda. <sup>[2]</sup> 2. To determine the percentage purity of a sample by titration. <sup>[2]</sup> 3. To determine the amount of nitrite present in the given water sample <sup>[2]</sup>

## Semester – II

### Paper I

#### Physical Chemistry:

Course Code: PGCH 201

(60 L)

#### Unit I

#### Chemical Thermodynamics II [15 L]

- 1.1. 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.
- 1.2. **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.
- 1.3. **Thermodynamics of surfaces,** Pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).
- 1.4. 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]

- 2.1. Rigid rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the  $\phi$  equation, wave function, quantum number, the  $\theta$  equation, wave function, quantization of rotational energy, spherical harmonics.
- 2.2. Hydrogen atom, the two particle problem, separation of the energy as translational and potential, separation of variables, the  $R$  the  $\theta$  \* and the  $\phi$  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
- 2.3. 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.
- 2.4 Application of the Schrödinger equation to two electron system, limitations of the equation, need for the approximate solutions, methods of obtaining the approximate solution of the Schrödinger wave equation

## Unit III

### Chemical Kinetics and Molecular Reaction Dynamics [15 L]

- 3.1. **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
- 3.2. **Kinetics of reactions catalyzed by enzymes** -Michaelis-Menten analysis, Lineweaver-Burk and Eadie Analyses.
- 3.3. **Inhibition of Enzyme action:** Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.
- 3.4. **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.

## Unit IV

### Solid State Chemistry and Phase Equilibria [15 L]

## 4.1 : Solid State Chemistry

### 4.1.1. Recapitulation: Structures and Defects in solids.

#### Types of Defects and Stoichiometry

- a) Zero dimensional (point) Defects
- b) One dimensional (line) Defects
- c) Two dimensional (Planar) Defects

## 4.2 Phase equilibria

### 4.2.1. Recapitulation: Introduction and definition of terms involved in phase rule.

Thermodynamic derivation of Gibbs Phase rule.

### 4.2.2. Two component system:

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

### 4.2.3. Three component system

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

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

## 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. 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.
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.

## Paper I

### Physical Chemistry Practical

**Course Code: PGCHP 201**

**(60L)**

#### Non – Instrumental:

- 1) Polar plots of atomic orbitals such as  $1s$ ,  $2P_y$  and  $3d_z$  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.
- 5) Determine the Transition temperature of sodium Sulphate decahydrate by solubility 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.
- 5) To determine Hydrolysis constant of aniline hydrochloride by pH Measurements

**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.

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**Paper II**

**Inorganic Chemistry:**

**Course Code: PGCH 202**

**(60L)**

**Unit I**

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

1.1 Ligand substitution reactions of:

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

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

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

**Unit II**

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

- 2.1. Eighteen and sixteen electron rule and electron counting with examples.
- 2.2. Preparation and properties of the following compounds
  - (a) Alkyl and aryl derivatives of Pd and Pt complexes
  - (b) Carbenes and carbynes of Cr, Mo and W
  - (c) Alkene derivatives of Pd and Pt
  - (d) Alkyne derivatives of Pd and Pt
  - (e) Allyl derivatives of nickel

(f) 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 compound 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]

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

**3.2. 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.

**3.3. Case Studies:**

(a) Itai-itai disease for Cadmium toxicity,

(b) Arsenic Poisoning in the Indo-Bangladesh region.

**3.4. 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]

4.1. 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.

4.2. 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.

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

4.4. Nitrogen fixation-nitrogenase, hydrogenases

4.5. Metal ion transport and storage: Ionophores, transferrin, ferritin and Fe-S cluster

4.6. Medicinal applications of cis-platin and related compounds, Mechanism for anti-cancer activity of cis-platin

### References

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.
7. Bioinorganic Chemistry by J.L Lippard & Berg

## **Inorganic Chemistry Practical**

**Course Code: PGCHP 202**

**(60L)**

### **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.
- 5) Synthesis of tetrabutylammonium tribromide (TBATB)

### **Instrumentation**

- 1) Estimation of Copper using Iodometric method Potentiometrically.
- 2) Estimation of Fe<sup>+3</sup> solution using 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

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## Paper III

**Organic Chemistry:**  
**Course Code: PGCH 203**

**(60 L)**

### Unit-I

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

**1.1.1. 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

**1.1.2. 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.

**1.1.3.** 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.

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

**1.2.1. 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).

**1.2.2. 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 II

### Reactions and Rearrangements: (15 L)

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

- 2.1. Reactions:** Baylis-Hilman reaction, McMurry Coupling, Nef reaction, Passerini reaction.
- 2.2. Concerted rearrangements:** Hofmann, Curtius, Lossen, Schmidt, Wolff.
- 2.3. Cationic rearrangements:** Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.
- 2.4. Anionic rearrangements:** Brook, Neber, Von Richter, Wittig, Gabriel-Colman, .

## Unit III

### 3.1. Alkylation of Nucleophilic Carbon Intermediates: (7 L)

- 3.1.1. Generation of carbanion, kinetic and thermodynamic enolate formation, Regioselectivity in enolate formation, alkylation of enolates.
- 3.1.2. Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site of alkylation.
- 3.1.3. Alkylation of aldehydes, ketones, esters, amides and nitriles.
- 3.1.4. Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines and imines.
- 3.1.5. Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).



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

- 3.2.1. 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.
- 3.2.2. Addition reactions with amines and iminium ions; Mannich reaction.
- 3.2.3. Amine catalyzed condensation reaction: Knoevenagel reaction.

## **Unit-IV**

### **NMR spectroscopy and Mass spectrometry (15 L)**

- 4.1. 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.
- 4.2. <sup>13</sup>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.
- 4.3. Mass spectrometry:** Introduction to Mass spectra, Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, ortho effect.
- 4.4.** Structure determination involving individual or combined use of the above spectral techniques.

### **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, 6<sup>th</sup>

## **Organic Chemistry Practical**

**Course Code: PGCHP 203**

**(60L)**

### **Learning objectives**

1. To enhance the separation techniques for organic compounds
2. To understand solubility of organic compound in different solvents
3. Determination of type and functional group of the organic compound

### **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:**

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

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**Paper IV**

**Analytical Chemistry:**

**Course Code: PGCH 204**

**(60 L)**

**Unit I**

**Chromatography [15 L]**

- 1.1 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]
- 1.2 Concept of plate and rate theories in chromatography:** efficiency, resolution, selectivity and separation capability. Optimization of chromatographic conditions.[5 L]
- 1.3 Gas Chromatography:** Instrumentation of GC with special reference to sample injection systems – split/split less, column types, solid/ liquid stationary phases, column switching techniques, temperature programming, Thermionic and mass spectrometric detector, Applications. [3 L]
- 1.4 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

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

**2.2 Mass spectrometry:** instrumentation, ion sources for molecular studies, electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources. Applications.[6 L]

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

## Unit III

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

Introduction, Principle, Instrumentation and Applications of:

**3.1.1** Scanning Electron Microscopy (SEM)

**3.1.2** Scanning Tunneling Microscopy (STM)

**3.1.3** Transmission Electron Microscopy (TEM)

**3.1.4** Electron Spectroscopy (ESCA)

### 3.2- Atomic Spectroscopy– [6L]

**3.2.1** Atomic Spectroscopy– Introduction, Principle, Instrumentation and Applications.

**3.2.2** Advantages and Limitations of AAS

## Unit IV

### Electroanalytical Methods (Numericals are Expected)

#### 4.1 Ion selective potentiometry and Polarography: [10 L]

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

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

- a. **Electrogravimetry:** Introduction, principle, instrumentation, factors affecting the nature of the

deposit, applications.[3 L]

- b. **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 Arnika, 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.

### **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.
7. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

## **Analytical Chemistry Practical**

**Course Code: PGCHP 204**

**(60L)**

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.
9. Analysis of Salbutal sulphate from asthma inhaler by UV spectrophotometry.

### **References**

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 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

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

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