



**Janardan Bhagat Shikshan Prasarak Sanstha's**

**CHANGU KANA THAKUR  
ARTS, COMMERCE & SCIENCE COLLEGE,  
NEW PANVEL**

**(AUTONOMOUS COLLEGE)**

**Re-accredited 'A+' Grade by NAAC  
'College with Potential for Excellence' Status Awarded by UGC  
'Best College Award' by University of Mumbai**

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

**Programme: M.Sc.**

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

**Choice Based Credit, Grading and Semester System (60:40)**

**w.e.f. Academic Year 2019-2020**

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**Syllabus for Approval**

Sr. No.	Heading	Particulars
1	<b>Title of Course</b>	M.Sc.-I Chemistry
2	<b>Eligibility for Admission</b>	The B.Sc. degree examination of University of Mumbai with chemistry 6 units or 3 units or degree of any other university recognized as equivalent thereto.
3	<b>Passing marks</b>	Minimum D Grade or equivalent minimum marks for passing at the Graduation level.
4	<b>Ordinances/Regulations (if any)</b>	
5	<b>No. of Semesters</b>	One year/Two semester
6	<b>Level</b>	P.G. part-I
7	<b>Pattern</b>	Semester (60:40)
8	<b>Status</b>	Revised
9	<b>To be implemented from Academic year</b>	2019-2020

**Name of BOS Chairman: Dr. S. K. Patil**

**Signature of BOS Chairman:**

## **Preamble of the Syllabus:**

Master of Science (M.Sc.) in chemistry is a post-graduate course of department of chemistry, Changu Kana Thakur Arts, Commerce & Science college, New Panvel (Autonomous).

There are two P.G. programmes in Chemistry, namely M.Sc. programme in Organic Chemistry and M.Sc. programme in Analytical Chemistry. Both P.G. programmes are equivalent in all respect for employment and higher studies. Each of these two P.G. programmes shall extend over a period of two academic years comprising of four semesters. The syllabi and scheme of examinations of these two programmes are detailed below. The theory and practicals of courses of two Semesters of the two programmes are same. 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. Chemistry is important to the world economy as well. The developments in Chemistry during last few decades are phenomenal. It is also seen that these developments are crossing the traditional vertical 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 more or more based on deep understanding the chemical phenomena. The emerging Chemical Technologies are highly science based. 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.

### **Objectives of the Course:**

1. To develop laboratory competence in relating chemical structure to spectroscopic phenomena.
2. To demonstrate the ability to synthesize, separate and characterize compounds using published reactions, protocols, standard laboratory equipment, and modern instrumentation.
3. To provide the students with sound preparation for requirement of modern industry and provide competency in basic academic research as well as a cohesive, clearly structured overview of Chemistry

### **Course Outcome:**

1. Think critically and analyse chemical problems.
2. Present scientific and technical information resulting from laboratory experimentation in both written and oral formats.
3. Work effectively and safely in a laboratory environment.
4. Use technologies/instrumentation to gather and analyse data.
5. Work in teams as well as independently.
6. Apply modern methods of analysis to chemical systems in a laboratory setting.

## **M. Sc. Chemistry**

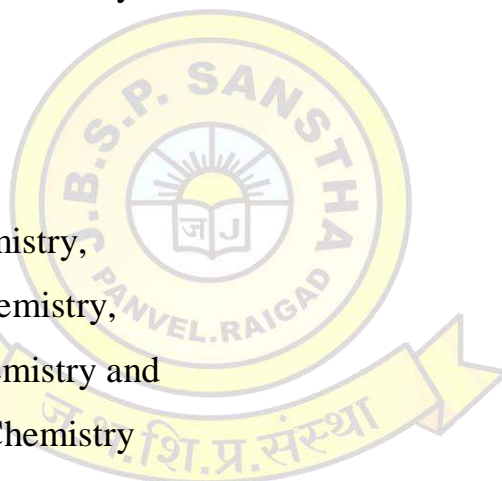
For the subject of chemistry there shall be four papers for 60 lectures each comprising of four units of 15 L each.

### **Semester-I**

1. Paper-I / Physical Chemistry,
2. Paper-II / Inorganic Chemistry,
3. Paper- III / Organic Chemistry and
4. Paper- IV /Analytical Chemistry

### **Semester-II**

1. Paper-I / Physical Chemistry,
2. Paper-II / Inorganic Chemistry,
3. Paper- III/ Organic Chemistry and
4. Paper- IV/ Analytical Chemistry



### ❖ Scheme of Examination

The performance of the learners shall be evaluated into two parts. The learner's performance shall be assessed by Internal Assessment with 40% marks in the first part and by conducting the Semester End Examinations with 60% marks in the second part. The allocation of marks for the Internal Assessment and Semester End Examinations are as shown below-

#### **A) Internal Assessment: 40 % 40 Marks**

Sr. No.	Particular	Marks
01	One periodical class test / online examination to be conducted in the given semester	20 Marks
02	One case study /review / project with presentation based on curriculum to be assessed by the teacher concerned	15 Marks
	Presentation	10 Marks
	Written Document	05 Marks
03	Active participation in routine class instructional deliveries and overall conduct as a responsible learner, mannerism and articulation and exhibit of leadership qualities in organizing related academic activities	05 Marks

### **Question Paper Pattern**

**(Periodical Class Test for the Courses at Under Graduate Programmes)**

Maximum Marks: 20

Duration: 40 Minutes

Questions to be set: 02

All Questions are Compulsory

Question No.	Particular	Marks
Q-1	Match the Column / Fill in the Blanks / Multiple Choice Questions/ Answer in One or Two Lines (Concept based Questions) ( 1 Marks / 2 Marks each)	10 Marks
Q-2	Answer in Brief (Attempt any Two of the Three) (5 Marks each)	10 Marks

## **B) Semester End Examination: 60 %**

**60 Marks**

- Duration: The examination shall be of 2  $\frac{1}{2}$  hours duration.

### ***Question Paper Pattern***

#### **Theory question paper pattern**

1. There shall be five questions each of 12 marks.
2. All questions shall be compulsory with internal options.
3. Question may be subdivided into sub-questions a, b, c... and the allocation of marks depends on the weightage of the unit.

#### **❖ Passing Standard**

The learners shall have to obtain a minimum of 40% marks in aggregate for each course where the course consists of Internal Assessment and Semester End Examination. The learners shall obtain minimum of 40% marks (i.e. 16 out of 40) in the Internal Assessment and 40% marks in Semester End Examination (i.e. 24 Out of 60) separately, to pass the course and minimum of grade D in each project wherever applicable to pass a particular semester.

#### **❖ Guidelines and Evaluation pattern for project work (100 Marks)**

##### **Introduction**

Inclusion of project work in the course curriculum of the M.Sc. programme is one of the ambitious aspects in the programme structure. The main objective of inclusion of project work is to inculcate the element of research work challenging the potential of learner as regards to his/ her eager to enquire and ability to interpret particular aspect of the study in his/ her own words. It is expected that the guiding teacher should undertake the counselling sessions and make the awareness among the learners about the methodology of formulation, preparation and evaluation pattern of the project work.

- There are two modes of preparation of project work
  1. Project work based on research methodology in the study area
  2. Project work based on internship in the study area

I	<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-1	From Unit – I (having internal options.) 12 M
	Q-2	From Unit – II (having internal options.) 12M
	Q-3	From Unit – III (having internal options.) 12M
	Q-4	From Unit – IV(having internal options.) 12M
	Q-5	Questions from all the FOUR Units with equal weightage of marks allotted to each Unit. 12 M
II	<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 External 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 (CBCGS)  
To be implemented from the Academic year 2019-2020**

**M.Sc.-I Chemistry  
Semester- I**

Course Code	Unit	Topics	Credits	L / Week
<b>PSC1CH1</b>	I	Thermodynamics-I	4	1
	II	Quantum Chemistry		1
	III	Chemical Dynamics-I		1
	IV	Electrochemistry		1
<b>PSC1CH2</b>	I	Chemical Bonding	4	1
	II	Molecular Symmetry and Group Theory		1
	III	Materials Chemistry and Nanomaterials		1
	IV	Characterisation of Coordination Compounds		1
<b>PSC1CH3</b>	I	Physical Organic Chemistry	4	1
	II	Nucleophilic substitution reactions and Aromaticity		1
	III	Stereochemistry		1
	IV	Oxidation and Reduction		1
<b>PSC1CH4</b>	I	Language of Analytical Chemistry	4	1
	II	Quality in Analytical Chemistry		1
	III	Optical Methods		1
	IV	Thermal Methods		1
<b>PSC1CH1 PSC1CH2 PSC1CH3 PSC1CH4</b>	-	Practical Course	8	16

**Choice Based Credit ,Grading and Semester System (CBCGS)  
To be implemented from the Academic year 2019-2020**

**M.Sc.-I Chemistry  
Semester- II**

Course Code	Unit	Topics	Credits	L / Week
<b>PSC2CH1</b>	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
<b>PSC2CH2</b>	I	Inorganic Reaction Mechanism	4	1
	II	Organometallic Chemistry of Transition metals		1
	III	Environmental Chemistry		1
	IV	Bioinorganic Chemistry		1
<b>PSC2CH3</b>	I	<ul style="list-style-type: none"> <li>• Alkylation of Nucleophilic Carbon Intermediates</li> <li>• Reaction of carbon nucleophiles with carbonyl groups</li> </ul>	4	1
	II	Reactions and Rearrangements		1
	III	<ul style="list-style-type: none"> <li>• Introduction to Molecular Orbital Theory for Organic Chemistry</li> <li>• Applications of UV and IR spectroscopy</li> </ul>		1
	IV	NMR spectroscopy and Mass spectrometry		1
<b>PSC2CH4</b>	I	Chromatography	4	1
	II	X-ray spectroscopy, Mass spectrometry, Radioanalytical Methods		1
	III	<ul style="list-style-type: none"> <li>• Surface Analytical Techniques</li> <li>• Atomic Spectroscopy</li> </ul>		1
	IV	Electroanalytical Methods		1
<b>PSC2CH1 PSC2CH2 PSC2CH3 PSC2CH4</b>	-	Practical Course	8	16

**Proposed Draft Syllabus For  
M.Sc. Chemistry  
Semester I and II  
Choice Based Credit System  
(To be implemented from the academic year, 2019-2020)  
Semester – I**

**Paper I**

**Physical Chemistry: Course Code: PSC1CH1 [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]

[Ref 2 and 1,10,11,12 17]

**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 and Hermitian operators, 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.

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]**

##### 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.

[Ref. 2 and 15, 17, 18]

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

4.4. 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. Goldman 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, 7th Edn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, Physical Chemistry, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, Physical Chemistry, 3rd Edn., John Wiley and Sons (Asia) Pte.Ltd., 2002.
4. Ira R. Levine, Physical Chemistry, 5th Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, Physical Chemistry, 3rd Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, Text Book of Physical Chemistry, 2nd 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, 2nd 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, 5th Edn., Pearson Education (Singapore) Pte.Ltd., Indian Branch, New Delhi, 2000.
14. Thomas Engel and Philip Reid, Physical Chemistry, 3rd Edn., Pearson Education Limited 2013.

15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st 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, 2nd Edn

## Physical Chemistry Practical

### Paper I

Course Code: **PSC1CH1**

#### 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  $\text{Ca(OH)}_2$  in presence of  $\text{NaOH}$  and hence to determine the solubility product of  $\text{Ca(OH)}_2$  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, 3rd 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: PSC1CH2 (60 L)**

### Unit I

#### Chemical Bonding: [15 L]

1.1 Recapitulation of hybridization Derivation of wave functions for sp, sp<sup>2</sup>, sp<sup>3</sup> orbital hybridization types considering only sigma bonding.

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

1.3 Molecular Orbital Theory for Polyatomic species considering  $\sigma$  bonding for SF<sub>6</sub>, CO<sub>2</sub>, B<sub>2</sub>H<sub>6</sub>, I<sub>3</sub><sup>-</sup> molecular species.

1.4 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<sub>2v</sub>, C<sub>3v</sub> and D<sub>2h</sub>, 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<sub>n</sub> (Ammonia, CH<sub>4</sub>) molecule.

(b) Determination of symmetry species for translations and rotations.

(c) Mulliken's notations for irreducible representations.

(d) Reduction of reducible representations using reduction formula.

(e) Group-subgroup relationships.

(f) Descent and ascent in symmetry correlation diagrams showing relationship between different groups.

### **Unit-III**

#### **Materials Chemistry and Nanomaterials: [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, Langmuir Blodgett(L-B) method, Biological methods: Synthesis using microorganisms.

3.2.2. Applications in the field of semiconductors, solar cells

### **Unit - IV**

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

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

4.2. Spectral calculations using Orgel and Tanabe-Sugano diagram, calculation of electronic parameters such as  $\Delta$ , B, C, 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, 2nd 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, 2nd Edition 2005.
5. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry—Principles of Structure and Reactivity, 4th 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, 3rd 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, 2nd 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, 2nd Edition, New Age International Publishers, New Delhi, 2009.
5. A. SalahuddinKunju 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. Banerjea ,Coordination Chemistry
3. Geary Coordination reviews
4. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver & Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.
5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th 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: PSC1CH2**

Inorganic Preparations (Synthesis and Characterization)

- 1) Bis-(tetraethylammonium) tetrachloroCuprate (II)  $(Et_4 N)_2[CuCl_4]$
  - 2) Bis-(tetraethylammonium) tetrachloroNickelate (II)  $(Et_4 N)_2 [NiCl_4]$
  - 3) Bis-(tetraethylammonium) tetrachloroCobaltate (II)  $(Et_4 N)_2 [CoCl_4]$
- (Any two from above preparations)
- 4) Tetramminemonocarbonato Cobalt (III) Nitrate  $[Co(NH_3)_4CO_3]NO_3$

5) Bis (ethylenediammine) Copper (II) Sulphate  $[\text{Cu}(\text{en})_2]\text{SO}_4$

6) Hydronium dichlorobis(dimethylglyoximate) Cobaltate(III)  $[\text{Co}(\text{dmgH})_2\text{Cl}_2] \text{H}^+$

### **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.

### **Reference:**

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st 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: PSC1CH3**

**Lectures: 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 and solvation. Comparative study of acidity and basicity of organic compounds on the basis of  $\text{pK}_a$  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**

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

2.1.1. Aliphatic nucleophilic substitution:  $S_N1$ ,  $S_N2$ ,  $S_Ni$  reactions, mixed  $S_N1$  and  $S_N2$  and SET mechanisms.  $S_N$  reactions involving NGP - participation by aryl rings,  $\alpha$ - and  $\pi$ -bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles.  $S_NcA$ ,  $S_N1''$  and  $S_N2''$  reactions.  $S_N$  at  $sp^2$  (vinylic) carbon.

2.1.2. Aromatic nucleophilic substitution:  $S_NAr$ ,  $S_N1$ , benzyne mechanisms. Ipso, cine, tele and vicarious substitution.

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

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

2.2.3. 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 L)

3.1. Concept of Chirality: Recognition of symmetry elements.

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

3.3. 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.

3.4. 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.

3.5. 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)

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

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  $HIO_4$ ; 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  $NaIO_4$ .

4.1.4. 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).

4.1.5. Oxidation of aldehydes and ketones: with  $H_2O_2$  (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 CO to  $CH_2$  in aldehydes and ketones- Clemmensen reduction, Wolff-Kishner reduction and Huang-Minlon modification.

4.2.2. 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).

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

4.2.4. 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.
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, PragatiPrakashan.

Organic Chemistry Practical

### Paper III

Course Code: **PSC1CH3**

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

#### Use of Computer - Chem Draw-Sketch, ISI – Draw:

Draw the structure of simple aliphatic, aromatic, heterocyclic organic compounds with substituents. Get the correct IUPAC name, Get  $^1\text{H}$ NMR and  $^{13}\text{C}$ . Students can able to draw the one name reaction and its reaction mechanism.

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: Course Code: **PSC1CH4**

Lectures: **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), philosophy implementation of TQM (reference of Kaizen, Six Sigma approach & 5S), 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), OSHA, Toxic Hazard (TH) classifications, Hazardous Chemical Processes (including process calorimetry / thermal build up concepts).

### **1.2.3 Accreditations:**

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

### **1.2.4 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.
- 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]**

##### 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, Drug analysis, Magnetic transition. e.g. Analysis of Polyethylene for its crystallinity.

##### **4.2 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, 5th Edition, Ch: 1. 3. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, 2004, Ch: 5. 4. Undergraduate Instrumental Analysis, 6th 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 ecotoxicological data". doi:10.1006/rtp.1996.1076. PMID 9056496.

## Unit II

1. 3000 solved problems in chemistry, Schaums Solved problem series, David E. Goldbers, McGraw 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, 5th Edition, Harcourt Asia Publisher. Chapter 6, 7.

2. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, 6th 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, 5th Edition, Harcourt Asia Publisher. Chapter 13, 14.

5. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, 6th 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, 5th 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, 5th 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, 7th Edition, Willard, Merrit, Dean: Chapter 25

4. Instrumental Analysis, 5th Edition, Skoog, Holler and Nieman: Chapter 31

5. Quantitative Chemical Analysis, 6 th 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 th Edition, Willard, Merrit, Dean: Chapter 26
8. Instrumental Analysis, 5th Edition, Skoog, Holler and Nieman: Chapter 33
9. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. GrawHill (1987): Chapter 28

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, 3rd 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 IntersciencePublication,New York,1978.

## **Semester – II**

### **Paper I**

**Physical Chemistry: Course Code: PSC2CH1**

**[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, wavefunction, 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  $\phi$  \* 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.

2.3. 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.

2.4. Hückel Molecular Orbitals theory for ethylene , 1,3-butadiene and benzene. (Derivation expected)

### **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.

(Ref: 7 and 2)

### **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

d) Thermodynamics of formation of defects (Mathematical derivation to find concentration of defects and numerical problems based on it)

(Ref: 17, 18 and 19 )

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

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

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

### References

1. Peter Atkins and Julio de Paula, Atkin's Physical Chemistry, 7th Edn., Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, Physical Chemistry, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, Physical Chemistry, 3rd Edn., John Wiley and Sons (Asia) Pte.Ltd., 2002.
4. Ira R. Levine, Physical Chemistry, 5th Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, Physical Chemistry, 3rd Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, Text Book of Physical Chemistry, 2nd Edn., McMillan and Co. Ltd., London, 1962.
7. Principles of Chemical Kinetics, 2nd 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, 2nd 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, 1972.
13. Peter A. Rock, Chemical Thermodynamics, University Science Books, Oxford University Press, 1983.

14. Ira N. Levine, Quantum Chemistry, 5th Edn., Pearson Education (Singapore) Pte.Ltd., Indian Branch, New Delhi, 2000.
15. Thomas Engel and Philip Reid, Physical Chemistry, 3rd Edn., Pearson Education Limited 2013.
16. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st 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 5th edition
22. Essentials of Physical Chemistry ,ArunBahl, 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: PSC2HP 201**

#### **Non – instrumental:**

1. Polar plots of atomic orbitals such as  $1s$ ,  $2p_x$  &  $3d_z^2$  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 dialtometric 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, 3rd 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: PSC2CH2**

#### Unit I

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

1.1 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).

1.2 Ligand substitution reactions of:

a) Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method)

b) Square planar complexes, trans-effect, its theories and applications. Mechanism and factors affecting these substitution reactions.

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

1.4 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 transition metal 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 compounds:

Zeise's salt, bis(triphenylphosphine)diphenylacetylene platinum(0)  $[\text{Pt}(\text{PPh}_3)_2(\text{HC}\equiv\text{CPh})_2]$ , diallynickel(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 metallothionins

4.6. 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, 5th Ed., Oxford University Press, 2010.
2. D. Banerjea, Coordination Chemistry, Tata McGraw Hill, 1993.
3. W. H. Malik, G. D./Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8th 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, 2nd Ed., Kluwer Academic/ Plenum Publishers, 2002
6. Gurdeep Raj, Advanced Inorganic Chemistry-Vol.II, 12th Edition, Goel publishing house, 2012.
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, 2nd 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, 3rd 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, 2nd ed, New Age International Pvt Ltd, 2000.
3. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5th edition, Wiley International Pvt, Ltd 2000.
4. B.Douglas, D.H McDaniel and J.J Alexander. Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley and Sons. 1983.
5. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.

### **Unit III**

1. Environmental Chemistry 5th edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.
2. Environmental Chemistry 7th edition, Stanley E. Manahan, CRC Press Publishers,
3. Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.
4. Environmental Science 13th 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 4th edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor & Francis Group, 2013.
6. Living in the Environment 17th 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 6th 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, California, 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 Fe<sup>+3</sup> solution using Ce(IV) ions Potentiometrically

#### **Reference:**

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st 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: PSC2CH3**

#### **Lectures 60 L**

#### **Unit-I**

- 1.1. Alkylation of Nucleophilic Carbon Intermediates: (7 L)

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

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

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

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

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

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

1.2.1. 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.

1.2.2. Addition reactions with amines and iminium ions; Mannich reaction.

1.2.3. Amine catalyzed condensation reaction: Knoevenagel reaction.

1.2.4. Acylation of carbanions.

[Reference Books: 1-11]

## **Unit II**

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

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

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

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

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

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

[Reference Books: 19-22]

## **Unit-III**

3.1. Introduction to Molecular Orbital Theory for Organic Chemistry: (7 L)

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

3.1.2. 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.

3.1.3. Application of FMO concepts in (a) SN2 reaction, (b) Lewis acid base adducts (BF<sub>3</sub>-NH<sub>3</sub> complex), (c) ethylene dimerization to butadiene, (d) Diels-Alder cycloaddition, (e) regioselective reaction of allylcation with allyl anion (f) addition of hydride to formaldehyde.

3.2. Applications of UV and IR spectroscopy: (8 L)

3.2.1. 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).

3.2.2. 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-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.  $^{13}\text{C}$  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.

4.3. 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.

4.4. 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 (7th 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
12. Molecular Orbital and Organic chemical reactions, Ian Fleming Reference Edition, Wiley



13. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.
14. Spectrometric Identification of Organic Compounds, R. Silverstein, G.C Bassler and T.C. Morrill, John Wiley and Sons.
15. Organic Spectroscopy, William Kemp, W.H. Freeman & Company.
16. Organic Spectroscopy-Principles and Applications, Jagmohan, Narosa Publication.
17. Organic Spectroscopy, V.R. Dani, Tata McGraw Hill Publishing Co.
18. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Ltd.
19. Organic Reaction Mechanisms, V.K. Ahluwalia, R.K. Parasher, Alpha Science International, 2011.
20. Reactions, Rearrangements and Reagents by S. N. Sanyal
21. Name Reactions, Jie Jack Li, Springer
22. Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, M.G. Eller, and F.G. Favalaro, John Wiley & Sons.

### **Organic Chemistry Practical**

#### **Paper III**

**Course Code: PSC2CH3**

#### **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: PSC2CH4**

**[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. Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions.[5 L]

1.3 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]

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: 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]

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 Electron Spectroscopy (ESCA and Auger)

#### 3.2 Atomic Spectroscopy [6 L]

##### 3.2.1 Advantages and Limitations of AAS

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

### **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), 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.

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

4.3 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 nd 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, 5th Edition, Ch: 12 4. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5th 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, 5th 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: **PSC2CH4**

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. Vogels, 3rd 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

UNIVERSITY OF MUMBAI



Janardan Bhagat Shikshan Prasarak Sanstha's

**Changu Kana Thakur**

**Arts, Commerce and Science College, New Panvel (Autonomous)**

Re-accredited A<sup>+</sup> Grade by NAAC

'College with Potential for Excellence' Status Awarded by UGC

'Best College Award' by University of Mumbai

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**Programme: M.Sc.**

(Choice Based Credit System)

**Course: Organic Chemistry**

**Programme Code: MSCOC1018**

**Syllabus for Semester III and IV**

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

### **Preamble of the Syllabus:**

Master of Science (M.Sc.) in Organic Chemistry is a post-graduate course of Changu Kana Thakur Arts, Commerce and Science College, New Panvel (Autonomous).

The students pursuing this course would have to develop in depth understanding of various aspects of the subject. The new curriculum of M.Sc. Organic Chemistry offers the courses which will prepare the students for critical thinking, understanding of the concepts in depth and skills for employability. The learning outcome based approach is intended to provide a focused and outcome based syllabus with an agenda to structure the teacher-learning experiences in a more student centric manner. The course combines the opportunity for students to acquire knowledge of wide range of cutting-edge fields in chemistry with sessions on theory, practical, presentation and a project supervised by one of the teacher.

### **Objectives of the Course:**

1. Develop analytical thinking and apply the same for understanding principles, proposing mechanism and logical conclusions.
2. Comprehensive understanding of the interdisciplinary nature of Chemistry and emerging trends in Chemistry.
3. Competency in design and planning of synthesis and carry out with Good Laboratory Practices.
4. Access, search and use of chemical literature and acquiring necessary skills to succeed in research and advance studies.
5. Competency in handling instruments and interpretation of spectral data for structure determination of organic compounds.

Janardan Bhagat Shikshan Prasarak Sanstha's  
**Changu Kana Thakur**  
 Arts, Commerce and Science College, New Panvel (Autonomous)

**Draft Syllabus**  
**Syllabus for the M.Sc. Semester III and IV**  
 Credit Based Semester and Grading System  
**To be implemented from the academic year 2020-2021**  
**SEMESTER III**

Course Code	Unit	Topics	Credits	L/Week
PSC3TOC0	I	Organic Reaction Mechanisms	4	1
	II	Pericyclic Reactions		1
	III	Stereochemistry-I		1
	IV	Photochemistry		1
PSC3SOC0	I	Name reactions with mechanism and application	4	1
	II	Radicals in Organic Synthesis		1
	III	Enamines, Ylides and $\alpha$ -C-H functionalization		1
	IV	Metals / Non-metals in organic synthesis		1
PSC3NPS0	I	Natural products-I	4	1
	II	Natural products-II		1
	III	Advanced Spectroscopic Techniques-I		1
	IV	Advanced Spectroscopic Techniques -II		1
PSC3MBG0	I	Drug discovery, design and development	4	1
	II	Drug design, development and synthesis		1
	III	Biogenesis and biosynthesis of natural products		1
	IV	Green chemistry		1
PSC3BIC0	I	Biomolecules-I	4	1
	II	Biomolecules-II		1
	III	Biomolecules-III		1
	IV	Biomolecules-IV		1
PSC3TOP0 & PSC3SOP0		Practicals	4	8
PSC3NPP0 & (PSC3MBP0 or PSC3BIP0)		Practicals	4	8



### SEMESTER IV

Course Code	Unit	Topics	Credits	L/Week
PSC4TOC0	I	Physical Organic Chemistry	4	1
	II	Supramolecular Chemistry		1
	III	Stereochemistry-II		1
	IV	Asymmetric Synthesis		1
PSC4SOC0	I	Designing Organic Synthesis-I	4	1
	II	Designing Organic Synthesis-II		1
	III	Electro-organic chemistry and selected methods of organic synthesis		1
	IV	Transition and rare earth metals in organic synthesis		1
PSC4NPH0	I	Natural products-III	4	1
	II	Natural products-IV		1
	III	Heterocyclic compounds-I		1
	IV	Heterocyclic compounds-II		1
PSC4IPR0	I	Introduction to Intellectual Property	4	1
	II	Trade Secrets		1
	III	Introduction to Cheminformatics		1
	IV	Applications		1
PSC4RMT0	I	Print	4	1
	II	Data Analysis		1
	III	Methods of scientific research and writing scientific papers		1
	IV	Chemical Safety & Ethical Handling of Chemicals		1
PSC4TOP0 & PSC4SOP0		Practicals	4	8
PSC4NPP0 & (PSC4IPP0 or PSC4RMP0)		Practicals	4	8

1. Credit based semester and grading system with effect from the academic year 2020-2021.
2. As per the credit system directives each credit will correspond to 15 hours of lectures or 30 hours of practical work.
3. Each student is expected to take 4 credits per theory paper and 2 credits per practical per semester.
4. At the end of each semester each student will be examined both in the theory and in the practical.
5. For the award of first class, the candidate must obtain at least 50% marks in the theory papers at the Semester I, II, III and IV of the M.Sc. examination taken together, in addition to the marks prescribed for the first class and the other rules of passing in the concerned regulation of the standard of passing.
6. The candidate is expected to submit a journal certified by the Head of the Department /institution at the time of the practical examination.
7. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
8. Use of non-programmable calculator is allowed both at the theory and the practical examination.

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### **Scheme of Examination for M.Sc. Organic Chemistry Semester III and IV**

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#### **Internal Theory examination (40 Marks)**

1. One class test **20 Marks**
2. One seminar based on curriculum / publication of a research paper/ presentation of a research paper in seminar or conference (to be assessed by teacher of the institution teaching PG learners). **15 Marks**
  - a) Selection of the topic, introduction, write up, references.
  - b) Presentation.
3. Active participation and overall conduct as a responsible learner in routine class, communication, and leadership qualities in organizing departmental academic activities. **05 Marks**

**There will not be any internal examination for practical.**

**External Theory Examination (60 Marks)**

<b>Paper</b>	<b>Time allotted in hours</b>	<b>Maximum marks</b>
Paper- I	2.5	60
Paper-II	2.5	60
Paper-III	2.5	60
Paper-IV	2.5	60

It is recommended that a total of five questions be set, based on the syllabus with due weightage to the number of lectures allotted per topic. The candidates are expected to answer all five questions. Question 5 will be based on all four units and the remaining questions will be based on the units as indicated below

<b>Question No.</b>	<b>Semester- III</b>	<b>Semester- III</b>
01	Unit I	Unit I
02	Unit II	Unit II
03	Unit III	Unit III
04	Unit IV	Unit IV
05	From all four units	From all four units

**Semester End Practical Examination (50 Marks)**

Laboratory Work **40 Marks**

Journal **05 Marks**

Viva **05 Marks**

The practical examination will be held for two days as described below. The candidates will be examined practically and orally on each day.

<b>Paper</b>	<b>Day</b>	<b>Experiments</b>	<b>Time duration in hours</b>	<b>Maximum marks</b>
I	Day-1 Morning	01	3.5	50
II	Day-1 Evening	01	3.5	50
III	Day-2 Morning	01	3.5	50
IV	Day-2 Evening	01	3.5	50

**M. Sc. Organic Chemistry**  
**Semester III**  
**Course Code - PSC3TOC0**  
**Paper I- Theoretical Organic Chemistry-I**

<b>Unit 1</b>	<b>Organic Reaction Mechanisms</b>	<b>15 L</b>
1.1	<b>Organic reactive intermediates:</b> Methods of generation, structure, stability and important reactions involving carbanions, carbocations, nitrenes, carbenes, arynes and ketenes.	<b>7L</b>
1.2	<b>Neighbouring group participation:</b> Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, $\pi$ -electrons, aromatic rings, $\sigma$ -bonds with special reference to norbornyl and bicyclo[2.2.2]octyl cation systems (formation of non-classical carbocation)	<b>4L</b>
1.3	<b>Role of FMOs in organic reactivity:</b> Reactions involving hard and soft electrophiles and nucleophiles.	<b>1L</b>
1.4	<b>Pericyclic reactions:</b> Recapitulation Explanations for Woodward-Hoffmann Rules <ul style="list-style-type: none"> <li>• The Aromatic Transition structures [Huckel and Mobius]</li> <li>• Frontier Orbitals</li> <li>• Correlation Diagrams, FMO and PMO approach</li> </ul> Molecular orbital symmetry, Frontier orbital of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system.	<b>3L</b>
<b>Unit 2</b>	<b>Pericyclic reactions</b>	<b>15L</b>
2.1	<b>Cycloaddition reactions:</b> Supra and antra facial additions, $4n$ and $4n+2$ Systems. Diels-Alder reactions (Diene, Dienophile, FMO approach, stereochemistry, endo rule, Intramolecular Diels-Alder reactions, regioselectivity/effect of substituents, Trapping of reactive intermediates), retro-Diels-Alder reaction. <b>2+2 Cycloadditions:</b> Photocycloadditions, Ketenes, 1,3-Dipolar cycloadditions and cheletropic reactions	<b>7L</b>
2.2	<b>Electrocyclic reactions:</b> Conrotatory and disrotatory motions, torquoselectivity, $(4n)$ $\pi$ and $(4n+2)$ $\pi$ electrons and allyl systems. Synthesis of endiandric acid A from an acyclic polyene.	<b>3L</b>
2.3	<b>Sigmatropic rearrangements:</b> H-shifts and C-shifts, supra and antarafacial migrations, Alder 'ene' Reaction, Cope (including oxy-Cope and aza-Cope), Claisen and Sommelet-Hauser rearrangements. Synthesis of Citral from 3-methylbut -2-en-1-ol and 3-methylbut-2-enal.	<b>5L</b>
<b>Unit 3</b>	<b>Stereochemistry-I</b>	<b>15L</b>
3.1	Conformational analysis of medium rings: Eight to ten membered rings and their unusual properties, I-strain, transannular reactions	<b>3L</b>
3.2	Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, perhydroanthracenes, steroids, and Bredt's rule.	<b>5L</b>
3.3	Anancomeric systems, Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): electrophilic addition, elimination, molecular rearrangements, reduction of cyclohexanones (with $\text{LiAlH}_4$ , selectride and MPV reduction) and oxidation of cyclohexanols.	<b>5L</b>

3.4	Stereospecific and Stereoselective reactions with specific examples	2L
<b>Unit 4</b>	<b>Photochemistry</b>	<b>15L</b>
4.1	<b>Principles of Photochemistry:</b> Recapitulation, Excited states and their properties, modes of dissipation of energy (Jablonski diagram), electronic energy transfer: photosensitization and quenching process, experimental set up for photochemical reactions.	3L
4.2	<b>Photochemistry of carbonyl compounds:</b> $\pi \rightarrow \pi^*$ , $n \rightarrow \pi^*$ transitions, Norrish- I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of $\alpha$ , $\beta$ -unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction.	7L
4.3	<b>Photochemistry of olefins:</b> cis-trans isomerizations, dimerizations, hydrogen abstraction, addition and Di- $\pi$ - methane rearrangement including oxa- di- $\pi$ --methane and aza-di- $\pi$ --methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes.	3L
4.4	<b>Photochemistry of arenes:</b> 1, 2-, 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings.	1L
4.5	Singlet oxygen and photo-oxygenation reactions. Photochemically induced Radical Reactions	1L

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**Course Code- PSC3SOC0**  
**Paper II - Synthetic Organic Chemistry -I**

<b>Unit 1</b>	<b>Name reactions with mechanism and application</b>	<b>15 L</b>
1.1	Mukaiyama esterification, Mitsunobu reaction, Darzen's Glycidic Ester Synthesis, Ritter reaction, Yamaguchi esterification, Peterson olefination.	5L
1.2	<b>Domino reactions:</b> Characteristics; Nazarov cyclization	3L
1.3	<b>Multicomponent reactions:</b> Strecker Synthesis, Ugi 4CC, Biginelli synthesis, Hantzsch synthesis, Pictet-Spengler synthesis	5L
1.4	<b>Click Reactions:</b> Characteristics; Huisgen 1,3-Dipolar Cycloaddition	2L
<b>Unit 2</b>	<b>Radicals in organic synthesis</b>	
2.1	<b>Introduction:</b> Generation, stability, reactivity and structural and stereochemical properties of free radicals, Persistent and charged radicals, Electrophilic and nucleophilic radicals.	3L
2.2	<b>Radical Initiators:</b> azobisisobutyronitrile (AIBN) and dibenzoyl peroxide.	1L
2.3	<b>Characteristic reactions:</b> Free radical substitution, addition to multiplebonds. Radical chain reactions, Radical halogenation of hydrocarbons (Regioselectivity), radical cyclizations, autoxidations: synthesis of cumene hydroperoxide from cumene.	4L
2.4	<b>Radicals in synthesis:</b> Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors. Cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling, C-C bond formation in aromatics: SRNAr reactions	4L
2.5	Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyer reaction, Acyloin condensation.	3L
<b>Unit 3</b>	<b>Enamines, Ylides and <math>\alpha</math>-C-H functionalization</b>	<b>15 L</b>
3.1	<b>Enamines:</b> Generation & application in organic synthesis with mechanistic pathways, Stork enamine reaction. Reactivity, comparison between enamines and enolates. Synthetic reactions of enamines including asymmetric reactions of chiral enamines derived from chiral secondary amines.	4L
3.2	<b>Phosphorus, Sulfur and Nitrogen Ylides:</b> Preparation and their synthetic applications along with their stereochemical aspects. Wittig reaction, Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination.	6L
3.3	<b><math>\alpha</math>-C-H functionalization:</b> By nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Bamford-Stevens reaction, Julia olefination and its modification, Seyferth-Gilbert homologation, Steven's rearrangement.	5L
<b>Unit 4</b>	<b>Metals / Non-metals in organic synthesis</b>	<b>15L</b>
4.1	<b>Mercury in organic synthesis:</b> Mechanism and regiochemistry of oxymercuration and demercuration of alkenes, mercuration of aromatics, transformation of aryl mercurials to aryl halides. Organomercurials as carbene transfer reagents.	3L
4.2	<b>Organoboron compounds:</b> Mechanism and regiochemistry of hydroboration of alkenes and alkynes, asymmetric hydroboration using chiral boron reagents, 9-BBN hydroboration, oxazaborolidine (CBS catalyst) and	3L

- functional group reduction by diborane.
- 4.3 Organosilicons:** Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allyl silanes.  $\beta$ -silyl cations as intermediates. Iodotrimethylsilane in organic synthesis. **3L**
- 4.4 Silyl enol ethers:** Application: As nucleophiles (Michael reaction, Mukaiyama aldol reaction), in ring contraction reactions. **2L**
- 4.5 Organotin compounds:** Preparation of alkenyl and allyl tin compounds; application in C-C bond formation, in replacement of halogen by H at the same C atom. **2L**
- 4.6 Selenium in organic synthesis:** Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno acetals as  $\alpha$ -C-H activating groups **2L**

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**Course code - PSC3NPS0**  
**Paper III- Natural products and Spectroscopy**

<b>Unit 1</b>	<b>Natural products-I</b>	<b>15 L</b>
1.1	<b>Carbohydrates:</b> Introduction to naturally occurring sugars: Deoxysugars, aminosugars, branched sugars. Structure elucidation of lactose and D-glucosamine (synthesis not expected). Structural features and applications of inositol, starch, cellulose, chitin and heparin.	<b>5L</b>
1.2	<b>Natural pigments:</b> General structural features, occurrence, biological importance and applications of: carotenoids, anthocyanins, quinones, flavones, pterins and porphyrins (chlorophyll). Structure elucidation of $\beta$ -carotene and Cyanin (with synthesis). Synthesis of ubiquinone from 3, 4, 5-trimethoxy methyl benzoate.	<b>5L</b>
1.3	<b>Terpenoids:</b> Occurrence, classification, structure elucidation, Stereochemistry, spectral data and synthesis of zingiberene. Synthesis of cinerolone, jasmolone and allethrolone.	<b>3L</b>
1.4	<b>Alkaloids:</b> Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine.	<b>2L</b>
<b>Unit 2</b>	<b>Natural products-II</b>	<b>15L</b>
2.1	<b>Multi-step synthesis of natural products:</b> Synthesis of the following natural products with special reference to reagents used, stereochemistry and functional group transformations: a) Woodward synthesis of Reserpine from benzoquinone b) Corey synthesis of Longifolene from resorcinol c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol d) Corey's Synthesis of Caryophyllene from 2-Cyclohexenone and Isobutylene e) Synthesis of Juvabione from Limonene f) Woodward synthesis of Strychnine	<b>10L</b>
2.2	<b>Prostaglandins:</b> Classification, general structure and biological importance. Structure elucidation of PGE <sub>1</sub> .	<b>2L</b>
2.3	<b>Insect Growth Regulators:</b> General idea, structures of JH <sub>2</sub> and JH <sub>3</sub> .	<b>1L</b>
2.4	<b>Plant Growth Regulators:</b> Structural features and applications of arylacetic acids, gibberellic acids and triacontanol. Synthesis of triacontanol (synthesis of stearyl magnesium bromide and 12-bromo-1-tetrahydropyranyloxydodecane expected)	<b>2L</b>
<b>Unit 3</b>	<b>Advanced Spectroscopic Techniques-I</b>	<b>15 L</b>
3.1	<b>Proton NMR spectroscopy:</b> Recapitulation, chemical and magnetic equivalence of protons, First order, second order, Spin system notations (A <sub>2</sub> , AB, AX, AB <sub>2</sub> , AX <sub>2</sub> , AMX and A <sub>2</sub> B <sub>2</sub> -A <sub>2</sub> X <sub>2</sub> spin systems with suitable examples). Long range coupling (Allylic coupling, 'W' coupling and Coupling in aromatic and hetero aromatic systems), Temperature effects, Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents.	<b>7L</b>
3.2	<b><sup>13</sup>C-NMR spectroscopy:</b> Recapitulation, equivalent and non-equivalent carbons (examples of aliphatic and aromatic compounds), <sup>13</sup> C- chemical shifts, calculation of <sup>13</sup> C- chemical shifts of aromatic carbons, heteronuclear coupling of carbon to <sup>19</sup> F and <sup>31</sup> P.	<b>4L</b>

3.3	Spectral problems based on UV, IR, <sup>1</sup> HNMR and <sup>13</sup> CNMR and Mass Spectroscopy.	4L
<b>Unit 4</b>	<b>Advanced Spectroscopic Techniques-II</b>	<b>15L</b>
4.1	<b>Advanced NMR techniques:</b> DEPT experiment, determining number of Attached hydrogens (methyl/methylene/methine and quaternary carbons), two dimensional spectroscopic techniques, COSY and HETCOR spectra, NOE and NOESY techniques.	10L
4.2	Spectral problems based on UV, IR, <sup>1</sup> HNMR, <sup>13</sup> CNMR (Including 2D technique) and Mass spectroscopy	5L

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**Course code - PSC3MBG0**  
**Paper IV- Medicinal, Biogenesis and Green Chemistry**

<b>Unit 1</b>	<b>Drug discovery, design and development</b>	<b>15 L</b>
1.1	<b>Introduction, important terms used in medicinal chemistry:</b> receptor, therapeutic index, bioavailability, drug assay and drug potency. General idea of factors affecting bioactivity: Resonance, inductive effect, bioisosterism, spatial considerations. Basic pharmacokinetics: drug absorption, distribution, metabolism (biotransformation) and elimination. Physical and chemical parameters like solubility, lipophilicity, ionization, pH, redox potential, H-bonding, partition coefficient and isomerism in drug distribution and drug-receptor binding.	<b>7L</b>
1.2	<b>Procedures in drug design:</b> Drug discovery without a lead: Penicillin, Librium. Lead discovery: random screening, non-random (or targeted) screening. Lead modification: Identification of the pharmacophore, Functional group modification. Structure-activity relationship, Structure modification to increase potency and therapeutic index: Homologation, chain branching, ring-chain transformation, bioisosterism, combinatorial synthesis (basic idea).	<b>8L</b>
<b>Unit 2</b>	<b>Drug design, development and synthesis</b>	<b>15L</b>
2.1	Introduction to quantitative structure activity relationship studies. QSAR parameters: - steric effects: The Taft and other equations; Methods used to correlate regression parameters with biological activity: Hansch analysis- A linear multiple regression analysis	<b>5L</b>
2.2	Introduction to modern methods of drug design and synthesis- computer aided molecular graphics based drug design, drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug design.	<b>3L</b>
2.3	Concept of prodrugs and soft drugs. (a) Prodrugs: Prodrug design, types of prodrugs, functional groups in prodrugs, advantages of prodrug use. (b) Soft Drugs: concept and properties.	<b>3L</b>
2.4	<b>Synthesis and application of the following drugs:</b> Fluoxetine, cetirizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol and Favipiravir Remdesivir: Structure and applications	<b>4L</b>
<b>Unit 3</b>	<b>Biogenesis and biosynthesis of natural products</b>	<b>15 L</b>
3.1	Primary and secondary metabolites and the building blocks, general pathway of amino acid biosynthesis.	<b>3L</b>
3.2	Acetate pathway: Biosynthesis of malonyl CoA, saturated fatty acids, prostaglandins from arachidonic acid, aromatic polyketides	<b>4L</b>
3.3	Shikimic Acid pathway: Biosynthesis of shikimic acid, aromatic amino acids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isoflavonoids.	<b>4L</b>
3.4	Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes-geranyl cation and its derivatives, sesquiterpenes-farnesyl cation and its derivatives and diterpenes.	<b>4L</b>
<b>Unit 4</b>	<b>Green chemistry</b>	<b>15L</b>
4.1	Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and	<b>1L</b>

	reaction conditions, green catalysts.	
<b>4.2</b>	<b>Use of the following in green synthesis with suitable examples:</b>	<b>9L</b>
	a) Green reagents: dimethylcarbonate, polymer supported reagents.	
	b) Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts [Aliquat 336, benzyltrimethyl ammonium chloride (TMBA), Tetra-n-butyl ammonium chloride, crown ethers], biocatalysts.	
	c) Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide.	
	d) Solid state reactions: solid phase synthesis, solid supported synthesis	
	e) Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions.	
	f) Ultrasound assisted reactions.	
<b>4.3</b>	Comparison of traditional processes versus green processes in the syntheses of ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene and benzimidazole.	<b>3L</b>
<b>4.4</b>	<b>Green Catalysts:</b> Nano catalyst, Types of Nano catalysts, Advantages and Disadvantages of Nano catalysts, Idea of Magnetically separable Nano catalysts.	<b>2L</b>

**Course code - PSC3BIC0**  
**Paper IV- Bioorganic Chemistry**

<b>Unit 1</b>	<b>Biomolecules-I</b>	<b>15 L</b>
<b>1.1</b>	<b>Amino acids, peptides and proteins:</b> Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, $\alpha$ - helix, $\beta$ -sheets, super secondary structure. Tertiary structure of protein: folding and domain structure. Quaternary structure.	<b>2L</b>
<b>1.2</b>	<b>Nucleic acids:</b> Structure and function of physiologically important nucleotides (c-AMP, ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation	<b>3L</b>
<b>1.3</b>	Structure: Purine & pyrimidine bases, ribose, deoxyribose, nucleosides and nucleotides (ATP, CTP, GTP, TTP, UTP) formation of polynucleotides strand with its shorthand representation.	<b>3L</b>
<b>1.4</b>	RNAs (various types in prokaryotes and eukaryotes) m- RNA and r- RNA— general account, t- RNA-clover leaf model, Ribozymes.	<b>2L</b>
<b>1.5</b>	<b>DNA:</b> Physical properties – Effect of heat on physical properties of DNA (Viscosity, buoyant density and UV absorption), Hypochromism, Hyperchromism and Denaturation of DNA. Reactions of nucleic acids (with DPA and Orcinol).	<b>2L</b>
<b>1.6</b>	<b>Chemical synthesis of oligonucleotides:</b> Phosphodiester, Phosphotriester, Phosphoramidite and H- phosphonate methods including solid phase approach	<b>3L</b>
<b>Unit 2</b>	<b>Biomolecules-II</b>	<b>15L</b>
<b>2.1</b>	<b>Chemistry of enzymes:</b> Introduction, nomenclature, classes and general types of reactions catalyzed by enzymes. Properties of enzymes: a) enzyme efficiency/ catalytic power b) enzyme specificity; Fischer's 'lock and key'	<b>6L</b>

	and Koshland ‘induced fit’ hypothesis. Concept and identification of active site.	
<b>2.2</b>	<b>Factors affecting enzyme kinetics:</b> Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and Irreversible inhibition.	<b>4L</b>
<b>2.3</b>	Mechanism of enzyme action: transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Mechanism of chymotrypsin catalyzed hydrolysis of a peptide bond	<b>5L</b>
<b>Unit 3</b>	<b>Biomolecules - III</b>	<b>15 L</b>
<b>3.1</b>	Chemistry of coenzymes. Structure, mechanism of action and bio-modeling studies of the following coenzymes: nicotinamide adenine dinucleotide, flavin adenine dinucleotide, thiamine pyrophosphate, pyridoxal phosphate, Vitamin B12, biotin, lipoic acid, Coenzyme A.	<b>12L</b>
<b>3.2</b>	Oxidative phosphorylation, chemiosmosis, rotary model for ATP synthesis and role of cytochrome in oxygen activation.	<b>3L</b>
<b>Unit 4</b>	<b>Biomolecules – IV</b>	<b>15L</b>
<b>4.1</b>	Role of main enzymes involved in the synthesis and breakdown of glycogen.	<b>2L</b>
<b>4.2</b>	Enzyme catalyzed organic reactions: Hydrolysis, hydroxylation, oxidation and reduction.	<b>6L</b>
<b>4.3</b>	Enzymes in organic synthesis. Fermentation: Production of drugs/drug intermediates by fermentation. Production of chiral hydroxy acids, vitamins, amino acids, $\beta$ -lactam antibiotics. Synthesis of chemicals via microbial transformation, synthesis of L-ephedrine. Chemical processes with isolated enzymes in free form (hydrocyanation of m-phenoxybenzaldehyde) and immobilized form (production of 6-aminopenicillanic acid).	<b>7L</b>

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15. Burger's medicinal chemistry and drug discovery. by Manfred E. Wolf
16. Introduction to Medicinal chemistry. by Graham Patrick
17. Medicinal chemistry-William O. Foye
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20. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R. Mahadik and K.G. Bothara , Nirali prakashan.
21. Medicinal chemistry (Vol. I and II)-Burger
22. Strategies for organic drug synthesis and design - D. Lednicer Wiley
23. Pharmacological basis of therapeutics-Goodman and Gilman's (McGraw Hill)
24. Enzyme catalysis in organic synthesis, 3rd edition. Edited by Karlheinz Drauz, Harold Groger, and Oliver May, Wiley-VCH Verlag GmbH & Co KgaA, 2012.
25. Biochemistry, Dr U Satyanarayan and Dr U Chakrapani, Books and Allied (P) Ltd.
26. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
27. The Organic Chemistry of Enzyme-Catalysed Reactions, Academic Press, By Richard B. Silverman
28. Enzymes: Practical Introduction to structure, mechanism and data analysis, By Robert A. Copeland, Wiley-VCH, Inc.
29. The Organic Chemistry of Biological Pathways By John McMurry, Tadhg Begley by Robert and company publishers
30. Bioorganic Chemistry- A practical approach to Enzyme action, H. Dugas and C. Penny. Springer Verlag, 1931
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35. Medicinal Natural Products: A Biosynthetic Approach by Paul M. Dewick. 3rd Edition, Wiley.
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41. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.

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  43. Organic synthesis in water. By Paul A. Grieco, Blackie.
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  45. New trends in green chemistry By V. K. Ahulwalia and M. Kidwai, 2<sup>nd</sup> edition, Anamaya Publishers, New Delhi.
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### **Semester III: Practicals**

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#### **Course code: PSC3TOP0 & PSC3SOP0**

#### **Separation of a ternary mixture of organic compounds and identification including derivative preparations using micro-scale technique (Minimum 8 experiments)**

1. Separation of a ternary mixture (S-S-S, S-S-L, S-L-L and L-L-L) (for solid mixture: water insoluble/ soluble including carbohydrates) based upon differences in the physical and the chemical properties of the components.
2. Identification of the two components (indicated by the examiner) using micro-scale technique.
3. Preparation of derivatives (any one of separated compound).

#### **Course code: PSC3NPP0 & (PSC3MBP0 or PSC3BIP0)**

#### **Single step organic preparation (1.0 g scale) involving purification by Steam distillation / Vacuum distillation or Column chromatography (Minimum 8 experiments)**

1. Preparation of acetanilide from aniline and acetic acid using Zn dust. (Purification by column chromatography)
2. Preparation of 1-nitronaphthalene from naphthalene. (Purification by steam distillation)
3. Preparation of acetyl ferrocene from ferrocene. (Purification by column chromatography)
4. Preparation of 3-nitroaniline from 1, 3-dinitrobenzene. (Purification by column chromatography)
5. Preparation of benzyl alcohol from benzaldehyde. (Purification by vacuum distillation).
6. Preparation of methyl salicylate from salicylic acid. (Purification by vacuum distillation).
7. Preparation of 4-methylacetophenone from toluene. (Purification by vacuum distillation).
8. Preparation of phenyl acetate from phenol. (Purification by vacuum distillation)
9. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation)
10. Preparation of fluorenone from fluorene. (Purification by column chromatography)
11. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation)



**Note:**

1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
2. Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

**References for Practicals:**

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
5. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
10. Vogel's Textbook of Practical Organic Chemistry, Fifth edition, 2008, B.S.Furniss, A. J.Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education.
11. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
12. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4<sup>th</sup> ed., 2011.

**Important Note:**

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

## Semester IV

### Course Code - PSC4TOC0

### Paper I- Theoretical Organic Chemistry-II

<b>Unit 1</b>	<b>Physical Organic Chemistry</b>	<b>15 L</b>
1.1	Structural effects and reactivity: Linear free energy relationship (LFER) in determination of organic reaction mechanism: The Hammett equation, Substituent constant ( $\sigma$ ) and $\sigma$ values, Reaction constants ( $\rho$ ), reactions with positive and negative $\rho$ values, Nonlinear Hammett plots (concave upwards and downwards deviations)	9L
1.2	Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants, Calculation of $k$ values, Taft equation, Solvent effects, Grunwald-Winstein equation, Dimroth's ET parameter, Spectroscopic correlations, Thermodynamic implications.	6L
<b>Unit 2</b>	<b>Supramolecular chemistry</b>	<b>15L</b>
2.1	Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.	3L
2.2	Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.	3L
2.3	Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes	5L
2.4	Molecular recognition and catalysis, molecular self-assembly. Supramolecular Polymers, Gels and Fibers.	4L
<b>Unit 3</b>	<b>Stereochemistry- II</b>	<b>15L</b>
3.1	Racemization and resolution of racemates including conglomerates: Mechanism of racemization, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds with stereospecific reactions.	3L
3.2	Determination of enantiomer and diastereomer composition: enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR).	3L
3.3	Correlative method for configurational assignment: chemical, optical rotation, and NMR spectroscopy.	4L
3.4	Molecular dissymmetry and chiroptical properties: Linearly and circularly polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial $\alpha$ -haloketone rule with applications.	5L
<b>Unit 4</b>	<b>Asymmetric Synthesis</b>	<b>15L</b>
4.1	Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions	3L
4.2	Synthesis of L-DOPA [Knowles's Monsanto process]. Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharpless enantioselective epoxidation, hydroxylation,	9L

aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.

- 4.3** Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations **3L**

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2. A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi.
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4. Mechanism and theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.
5. Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.
6. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan Publishers, India.
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12. Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
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15. Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.
16. Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
17. Pericyclic reactions, Ian Fleming, Oxford University press, 1999.
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19. Organic chemistry, 8th edition, John McMurry
20. Modern methods of Organic Synthesis, 4th Edition W. Carruthers and Iain Coldham, Cambridge University Press 2004

21. Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books, 2006
22. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
23. Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3<sup>rd</sup> edition, New Age International Ltd.
24. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit
25. Stereochemistry, P. S. Kalsi, 4<sup>th</sup> edition, New Age International Ltd
26. Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
27. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
28. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
29. Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
30. Large ring compounds, J.A. Semlyen, Wiley-VCH, 1997.
31. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley-Eastern
32. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
33. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
34. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
35. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
36. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
37. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A John Wiley and Sons, Ltd., Publication)

**Course Code- PSC4SOC0**  
**Paper II- Synthetic Organic Chemistry-II**

<b>Unit 1</b>	<b>Designing Organic Synthesis-I</b>	<b>15 L</b>
1.1	Protecting groups in Organic Synthesis: Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.	3L
1.2	Concept of umpolung (Reversal of polarity): Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.	3L
1.3	Introduction to Retrosynthetic analysis and synthetic planning: Linear and convergent synthesis; Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions (FGI), functional group addition (FGA), functional group removal (FGR) importance of order of events in organic synthesis, one and two group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds), selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity	9L

<b>Unit 2</b>	<b>Designing Organic Synthesis-II</b>	<b>15L</b>
2.1	General strategy: choosing a disconnection-simplification, symmetry, high yielding steps, and recognisable starting material.	3L
2.2	One group C-C Disconnections: Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.	6L
2.3	Two group C-C Disconnections: 1,2- 1,3- 1,4- 1,5- and 1,6-difunctionalized compounds, Diels-Alder reactions, $\alpha$ , $\beta$ -unsaturated compounds, control in carbonyl condensations, Michael addition and Robinson annelation.	6L
<b>Unit 3</b>	<b>Electro-organic chemistry and Selected methods of Organic synthesis</b>	<b>15L</b>
3.1	<b>Electro-organic chemistry:</b> <b>Introduction:</b> Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes. <b>Cathodic reduction:</b> Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins, arenes, electro-dimerization. <b>Anodic oxidation:</b> Oxidation of alkylbenzene, Kolbe reaction, Non-Kolbe oxidation, Shono Oxidation	7L
3.2	<b>Selected Methods of Organic synthesis</b> Applications of the following in organic synthesis: <ul style="list-style-type: none"> <li>• Crown ethers, cryptands, micelles, cyclodextrins, catenanes.</li> <li>• Organocatalysts: Proline, Imidazolidinone.</li> <li>• Pd catalysed cycloaddition reactions: Stille reaction, Saegusa-Ito oxidation to enones, Negishi coupling.</li> <li>• Use of Sc(OTf)<sub>3</sub> and Yb(OTf)<sub>3</sub> as water tolerant Lewis acid catalyst in aldol condensation, Michael reaction, Diels-Alder reaction, Friedel – Crafts reaction.</li> </ul>	8L
<b>Unit 4</b>	<b>Transition and rare earth metals in organic synthesis</b>	<b>15L</b>
4.1	<b>Introduction to basic concepts:</b> 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion.	3L
4.2	Palladium in organic synthesis: $\pi$ -bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerisation, cross-coupling of organometallics and halides. Representative examples: Heck reaction, Suzuki-Miyaura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S, or P atoms.	5L
4.3	Olefin metathesis using Grubb's catalyst.	1L
4.4	Application of Ni, Co, Fe, Rh, and Cr carbonyls in organic synthesis.	4L
4.5	Application of samarium iodide including reduction of organic halides, aldehydes and ketones, $\alpha$ -functionalised carbonyl and nitro compounds.	1L
4.6	Application of Ce (IV) in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent.	1L

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1. Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5<sup>th</sup> Edition, Springer Verlag
2. Modern Methods of Organic Synthesis, 4<sup>th</sup> Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
3. Chem. Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam.
4. Organic Chemistry, Clayden Greeves Warren and Wothers, Oxford Press (2001).
5. Modern Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
6. Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002).
7. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3<sup>rd</sup> Edn., Nelson Thornes
8. Organic Chemistry, 7<sup>th</sup> Edn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson
9. Strategic Applications of Name Reactions in Organic Synthesis, L. Kurti & B. Czako (2005), Elsevier Academic Press
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13. Name Reactions and Reagents in Organic Synthesis, 2<sup>nd</sup> Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
14. Name Reactions, Jie Jack Lie, 3<sup>rd</sup> Edn., Springer
15. Organic Electrochemistry, H. Lund, and M. Baizer, 3<sup>rd</sup> Edn., Marcel Dekker.

### Course Code- PSC4NPH0

#### Paper III- Natural products and Heterocyclic Chemistry

<b>Unit 1</b>	<b>Natural products-III</b>	<b>15 L</b>
<b>1.1</b>	<b>Steroids:</b> General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following: corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bile acids.	<b>5L</b>
<b>1.2</b>	Synthesis of 16-DPA from cholesterol and plant sapogenin.	<b>2L</b>
<b>1.3</b>	Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone.	<b>5L</b>
<b>1.4</b>	<b>Insect pheromones:</b> General structural features and importance. Types of pheromones (aggregation, alarm, releaser, primer, territorial, trail, sex pheromones etc.), advantage of pheromones over conventional pesticides. Synthesis of bombykol from acetylene, dispartlure from 6-methylhept-1-ene, grandisol from 2-methyl-1, 3-butadiene.	<b>3L</b>

<b>Unit 2</b>	<b>Natural products-IV</b>	<b>15L</b>
<b>2.1</b>	<b>Vitamins:</b> Classification, sources and biological importance of vitamin B <sub>1</sub> , B <sub>2</sub> , B <sub>6</sub> , folic acid, B <sub>12</sub> , C, D <sub>1</sub> , E ( $\alpha$ -tocopherol), K <sub>1</sub> , K <sub>2</sub> , H ( $\beta$ - biotin). Synthesis of the following: Vitamin A from $\beta$ -ionone and bromoester moiety. Vitamin B <sub>1</sub> including synthesis of pyrimidine and thiazole moieties Vitamin B <sub>2</sub> from 3, 4-dimethylaniline and D(-) ribose Vitamin B <sub>6</sub> from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethyl ester of N-formyl-DL-alanine (Harris synthesis) Vitamin E ( $\alpha$ -tocopherol) from trimethylquinol and phytol bromide Vitamin K <sub>1</sub> from 2-methyl-1, 4-naphthaquinone and phytol	<b>6L</b>
<b>2.2</b>	<b>Antibiotics:</b> Classification on the basis of activity. Structure elucidation, spectral data of penicillin-G and chloramphenicol. Synthesis of chloramphenicol (from benzaldehyde and $\beta$ -nitroethanol) penicillin-G and phenoxymethylpenicillin from D-penicillamine and t-butyl phthalimide malonaldehyde (synthesis of D-penicillamine and t-butyl phthalimide malonaldehyde expected).	<b>6L</b>
<b>2.3</b>	<b>Naturally occurring insecticides:</b> Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis of pyrethrin I.	<b>2L</b>
<b>2.4</b>	Synthesis of exaltone and muscone.	<b>1L</b>
<b>Unit 3</b>	<b>Heterocyclic compounds-I</b>	<b>15L</b>
<b>3.1</b>	Heterocyclic compounds: Introduction, classification, Nomenclature of heterocyclic compounds of monocyclic (3-6 membered) (Common, systematic (Hantzsch-Widman ) and replacement nomenclature)	<b>3L</b>
<b>3.2</b>	Structure and nucleophilic ring opening reactions of aziridines, oxiranes, oxetanes and azetidines	<b>2L</b>
<b>3.3</b>	Structure, reactivity, synthesis and reactions of pyridine, pyridine N-oxide, pyridazine, pyrimidine, pyrazine, pyrrole, pyrazoles, Imidazoles, thizoles and oxazoles	<b>10L</b>
<b>Unit 4</b>	<b>Heterocyclic compounds-II</b>	<b>15L</b>
<b>4.1</b>	Nomenclature of heterocyclic compounds of bicyclic/tricyclic (5-6 Membered) fused heterocycles (up to three hetero atoms). (Common, systematic (Hantzsch-Widman) and replacement nomenclature)	<b>3L</b>
<b>4.2</b>	Structure, reactivity, synthesis and reactions of quinoline, isoquinoline, indole, coumarines, purines, benzimidazoles, benzthiazoles, quinoxaline, cinnoline and quinazoline	<b>12 L</b>

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1. Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B.G. Torssell, Apotekarsocieteten –Swedish Pharmaceutical Press.
2. Natural products chemistry and applications, Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House, 2011.
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6. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co. 2008.
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10. Heterocyclic Chemistry, J. A. Joule and G. F. Smith, ELBS, 2<sup>nd</sup> edition, 1982.
11. The Conformational Analysis of Heterocyclic Compounds, F.G. Riddell, Academic Press, 1980.
12. Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978.
13. An Introduction to the Chemistry of Heterocyclic Compounds, 2<sup>nd</sup> edition, B.M. Acheson, 1975.
14. Natural Products: Chemistry and Biological Significance Interscience, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J. B. Harborne, Longman, Essex, 1994.
15. Organic Chemistry, Vol 2, I.L. Finar, ELBS, 6<sup>th</sup> edition, Pearson.
16. Stereoselective Synthesis: A Practical Approach, M. Nogradi, Wiley-VCH, 1995.
17. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
18. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
19. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers, 1998.
20. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers, 1998.
21. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.
22. Comprehensive Organic Chemistry by Barton and Ollis, Pergamon Press, Oxford, 1979.
23. Medicinal Natural Products, a Biosynthetic Approach, Derick Paul, John Wiley and Sons, 2002.
24. Biosynthesis of Natural Products, Mannitto Paolo, Ellis Horwood Limited, 1981.
25. Selected Organic synthesis, Ian Fleming, John Wiley and Sons, 1973.

### **Course Code- PSC4IPR0**

#### **Paper IV- Intellectual Property Rights & Cheminformatics**

<b>Unit 1</b>		<b>15 L</b>
<b>1.1</b>	<b>Introduction to Intellectual Property:</b> Historical Perspective, Different types of IP, Importance of protecting IP.	<b>2L</b>
<b>1.2</b>	<b>Patents:</b> Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.	<b>5L</b>
<b>1.3</b>	<b>Industrial Designs:</b> Definition, How to obtain, features, International design registration.	<b>2L</b>



1.4	<b>Copyrights:</b> Introduction, How to obtain, Differences from Patents.	2L
1.5	<b>Trade Marks:</b> Introduction, How to obtain, Different types of marks– Collective marks, certification marks, service marks, trade names etc.	2L
1.6	<b>Geographical Indications:</b> Definition, rules for registration, prevention of illegal exploitation, importance to India.	2L
<b>Unit 2</b>		<b>15L</b>
2.1	<b>Trade Secrets:</b> Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.	2L
2.2	<b>IP Infringement issue and enforcement:</b> Role of Judiciary, Role of law enforcement agencies-Police, Customs etc.	2L
2.3	<b>Economic Value of Intellectual Property:</b> Intangible assets and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.	5L
2.4	<b>Different International agreements:</b>	6L
	<b>a. World Trade Organization (WTO):</b>	
	1. General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement	
	2. General Agreement on Trade Related Services (GATS) Madrid Protocol.	
	3. Berne Convention	
	4. Budapest Treaty	
	<b>b. Paris Convention</b>	
	<b>WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity.</b>	
<b>Unit 3</b>		<b>15L</b>
3.1	<b>Introduction to Cheminformatics:</b> History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.	5L
3.2	<b>Representation of molecules and chemical reactions:</b> Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.	5L
3.3	<b>Searching Chemical Structures:</b> Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.	5L
<b>Unit 4</b>	<b>Applications:</b>	<b>15L</b>
	Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand based and Structure based Drug design, Application of Cheminformatics in Drug Design.	

## REFERENCES:

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics*. Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley-VCH
3. Gupta, S. P. *QSAR and Molecular Modeling*. Springer-Anamaya Pub.: New Delhi.

## Course Code- PSC4RMT0 Paper IV- Research Methodology

<b>Unit 1</b>		<b>15 L</b>
<b>1.1</b>	<b>Print:</b> Primary, Secondary and Tertiary sources. <b>Journals:</b> Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.	<b>5L</b>
<b>1.2</b>	<b>Digital:</b> Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.	<b>5L</b>
<b>1.3</b>	<b>Information Technology and Library Resources:</b> The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.	<b>5L</b>
<b>Unit 2</b>	<b>DATA ANALYSIS</b>  <b>The Investigative Approach:</b> Making and recording Measurements, SI units and their use, Scientific methods and design of experiments. <b>Analysis and Presentation of Data:</b> Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis	<b>15L</b>
<b>Unit 3</b>	<b>METHODS OF SCIENTIFIC RESEARCH AND WRITING</b>	<b>15L</b>
<b>3.1</b>	<b>SCIENTIFIC PAPERS:</b> Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.	
<b>3.2</b>	<b>Writing Scientific Papers:</b> Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism	
<b>Unit 4</b>	<b>CHEMICAL SAFETY &amp; ETHICAL HANDLING OF CHEMICALS</b>  Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressure, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory	<b>15L</b>

chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

#### REFERENCES:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), *Practical skills in Chemistry*, 2<sup>nd</sup> Ed., Prentice Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) *Data Analysis for Chemistry* Oxford University Press.
3. Topping, J., (1984) *Errors of Observation and their Treatment* 4<sup>th</sup> Ed., Chapman Hill London.
4. Harris, D. C. (2007) *Quantative Chemical Analysis* 6<sup>th</sup> Ed., Freeman Chapters 3-5
5. Levie, R. De. (2001) *How to use Excel in Analytical Chemistry and in general scientific data analysis* Cambridge University Press.
6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

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### Semester IV: Practicals

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#### Course code: PSC4TOP0 & PSC4SOP0

##### Two steps preparations (Minimum 8 experiments)

1. Acetophenone → Acetophenone phenyl hydrazine → 2-phenyl indole.
2. 2-naphthol → 1-phenyl azo-2-naphthol → 1-amino-2-naphthol.
3. Cyclohexanone → cyclohexanone oxime → Caprolactum.
4. Hydroquinone → hydroquinone diacetate → 2,5-dihydroxyacetophenone.
5. 4-nitrotoluene → 4-nitrobenzoic acid → 4-aminobenzoic acid.
6. *o*-nitroaniline → *o*-phenylene diamine → Benzimidazole.
7. Benzophenone → benzophenone oxime → benzanilide.
8. *o*-chlorobenzoic acid → N-phenyl anthranilic acid → acridone.
9. Benzoin → benzil → benzilic acid.
10. Phthalic acid → phthalimide → anthranilic acid.
11. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-methyl-7-acetoxy Coumarin
12. Anthracene → anthraquinone → anthrone

#### Note:

1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
2. Students are expected to purify the product by recrystallization, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

## **Course code: PSC4NPP0 & (PSC4IPP0 or PSC4RMP0)**

### **Session-I:**

#### **Combined spectral identification: Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and Mass spectra).**

A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information should be reported within first half an hour of the examination without referring to any book/reference material. The complete structure of the compound may then be elucidated by referring to any standard text-book/reference material etc.

**(Minimum 8 spectral analysis)**

### **Session-II: Project evaluation OR Internship**

#### **References for Practicals:**

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V. K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
5. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
10. Vogel's Textbook of Practical Organic Chemistry, Fifth edition, 2008, B.S.Furniss, A. J.Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education.
11. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
12. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4<sup>th</sup> ed., 2011.

#### **Important Note:**

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.



Janardan Bhagat Shikshan Prasarak Sanstha's  
**CHANGU KANA THAKUR**  
**ARTS, COMMERCE & SCIENCE COLLEGE,**  
**NEW PANVEL (AUTONOMOUS)**  
Re-accredited 'A+' Grade by NAAC  
'College with Potential for Excellence' Status Awarded by UGC  
'Best College Award' by University of Mumbai

Programme: M.Sc.  
Course: M.Sc.-II  
Analytical Chemistry  
Choice Based Credit, Grading and Semester System (60:40)  
w.e.f. Academic Year 2020-2021

**Syllabus for Approval**

Sr. No.	Heading	Particulars
1	Title of Course	M.Sc.-I Chemistry
2	Eligibility for Admission	Passed from M.Sc. I
3	Passing marks	Minimum D Grade or equivalent minimum marks for passing at the Graduation level.
4	Ordinances/Regulations (if any)	
5	No. of Semesters	One year/Two semester
6	Level	P.G. part-II
7	Pattern	Semester (60:40)
8	Status	Revised
9	To be implemented from Academic year	2020-2021

**Name of BOS Chairman: Dr. S. K. Patil**

**Signature of BOS Chairman:**

## **Preamble of the Syllabus:**

Master of Science (M.Sc.) in analytical chemistry is a post-graduate course of department of chemistry, Changu Kana Thakur Arts, Commerce & Science college, New Panvel (Autonomous).

The programme is envisioned to provide a focused, outcome-based syllabus at the postgraduate level with student-centric structure of the teaching-learning experiences. It engages students in the curriculum of their choice and prepare students for both academia and employability.

The new curriculum of MSc II (Analytical Chemistry) offer courses in the various areas of analytical chemistry. All the courses are having defined objectives and Learning Outcomes, which will help prospective students in choosing the elective courses to broaden their skills in the field of chemistry and interdisciplinary areas.

The courses will train students with sound theoretical and experimental knowledge that suits the need of academics and industry. The courses also offers ample skills to pursue research as career in the field of chemistry and allied areas.

Department of Chemistry of Changu Kana Thakur Arts, Commerce and Science College hope the programme will create best analytical minds to meet the needs of society.

## **Objectives of the Course:**

1. To develop laboratory competence related instrumental and non-instrumental analysis
2. To demonstrate the ability of critical thinking and data analysis.
3. To provide the students with sound preparation for requirement of modern industry and provide competency in basic academic research as well as a cohesive, clearly structured overview of Chemistry

### **Course Outcomes**

#### **M. Sc. Part II Analytical Chemistry**

#### **Semester III**

#### **Paper 1: Theory**

- CSO1.** Students will understand theoretical aspects of sampling, pre-treatment and method validation.
- CSO2.** Student will get knowledge of how to measure uncertainty in measurements, dealing with signal to noise ratio and legislator aspects of pharmaceutical industries.
- CSO3.** Students will learn the principle of different separation techniques and their applications in various fields.
- CSO4.** Students will get detailed insights of modern chromatographic techniques for separation of mixture on the basis of charge, size, and affinity of composition.

### **Paper 1: Practical**

**CSO1.** Students will learn the instrument based analysis of various types of samples.

**CSO2.** Students will learn graphical representation of the data.

### **Paper 2: Theory**

**CSO1.** Student will help to understand the theoretical concepts of surface analytical techniques.

**CSO2.** Student will understand advanced spectroscopic techniques used for characterization of matter.

**CSO3.** Students will get detailed insights of advanced electroanalytical techniques.

**CSO4.** Student will find applications of chemiluminescence, ORD-CD, Photoacoustic spectroscopy in analytical chemistry.

### **Paper 2: Practical**

**CSO1.** Students will learn the various analytical techniques for pharmaceutical analysis.

**CSO2.** Students will get acquainted with the analysis of biological samples.

### **Paper 3: Theory**

**CSO1.** Student will learn bioanalytical techniques of analysis.

**CSO2.** Student will understand the immunological methods and the theoretical basic of each method.

**CSO3.** Student will get general idea about food processing, food preservation and determination of food contaminant etc.

**CSO4:** Student will understand technique use in food packaging and food analysis.

### **Paper 3: Practical**

**CSO1.** Students will perform practical's based upon food analysis

**CSO2:** Students will understand data acquisition and analysis.

### **Paper 4 E1: Theory**

**CSO1.** Student will learn different aspects of analysis of air pollutants.

**CSO2.** Student will understand the quality and requirement of potable water of bore well and bottle mineral water.

**CSO3.** Student will study the details of sources and hazardous of soil pollutant, noise pollutant, thermal pollutant, radioactive pollutant etc.

**CSO4.** Student will do the detail study of insecticides, pesticides, soaps, detergents and petrochemical products and their effects on environment.

### **Paper 4 E2: Theory**

**CSO1:** Student will get general idea regarding the pharmaceutical analysis and quality control methods of pharmaceutical industry.

**CSO2:** Student will know the details of drug analysis on the basis of functional groups and other factors.

**CSO3:** Student will understand the applications of analytical chemistry in forensic science.

**CSO4:** Student will learn the various aspects of cosmetic industry and analysis of different type cosmetics.

### **Paper 4: Practical**

**CSO1:** Students will perform the metallurgical analysis.

**CSO2.** Students will deal with the experiments related with environmental pollution.

## **Semester IV**

### **Paper 1: Theory**

**CSO1:** Student will learn details of various separation processes.

**CSO2.** Student will study the separation, analysis and standardization of herbal based products.

**CSO3.** Student will get conversant with the principle, advantages and challenges of green chemistry.

**CSO4.** Student will understand the concept of electrophoresis in analysis and basics of nanotechnology.

### **Paper 1: Practical**

**CSO1:** Student will understand the use of instrumental methods for the analysis of metallurgical samples as well as other samples.

### **Paper 2: Theory**

**CSO1:** Student will do the detail study of principle, instrumentation and applications of NMR spectroscopy.



- CSO2:** Student will understand the detail concept of mass spectroscopy and Raman spectroscopy.
- CSO3:** Student will learn principle and interfacing of radio analytical techniques and hyphenated thermal methods
- CSO4:** Student will know the detail concept of hyphenated techniques including GC-MS, GC-IR, LC-MS, HPLC-MS etc.

**Paper 2: Practical**

- CSO1:** Student will learn the quantitative estimation of pharmaceutical products.
- CSO2:** Students will get knowledge of quality control methods and understand the importance of accuracy.

**Paper 3: Theory**

- CSO1:** Student will learn the different aspects of effluent treatment.
- CSO2:** Student will understand steps involved in solid waste management.
- CSO3:** Student will get an idea about classifications and applications of plastics, polymer, paints and pigments and their environmental impact.
- CSO4:** Student will study metallurgical analysis.

**Paper 3: Practical**

- CSO1:** Students will learn quantitative estimation of various types of food samples.

**Paper 4E1: Theory**

- CSO1:** Student will learn about details intellectual property.
- CSO2:** Student will get knowledge of intellectual property rights (IPR).
- CSO3:** Student will understand concepts in cheminformatics.
- CSO4:** Student will learn the drug designing and traits in it.

**Paper 4E2: Theory**

- CSO1:** Student will learn every aspect of publication of research paper such as terms associated with journals, referencing and library resources.
- CSO2:** Student will get conversant with the methods of data analysis and various softwares employed for it.
- CSO3:** Student will get knowledge of actual writing scientific papers.
- CSO4:** Student will get information of the safety and ethical handling of chemicals.

**Paper 4: Practical**

- CSO1:** Student will actually get involved in research work.
- CSO2:** Student will understand the analysis of data generated by their research work.
- CSO3:** Student will learn how to present research work.

## **M. Sc. Analytical Chemistry**

For the subject of analytical chemistry there shall be four papers for 60 lectures each comprising of four units of 15 L each.

### **Semester-III**

1. Paper-I / Quality in Analytical Chemistry
2. Paper-II / Advanced Analytical Techniques
3. Paper- III / Bio-analytical Chemistry and Food Analysis
4. Paper- IV (Elective course-1)/ Environmental and Certain Industrially Important  
Materials  
(Elective course-2)/ Pharmaceutical and Organic Analysis

### **Semester-II**

1. Paper-I / Quality in Analytical Chemistry
2. Paper-II / Advanced Analytical Techniques
3. Paper- III/ Selected Topics in Analytical Chemistry
4. Paper- IV (Optional course-1)/ Intellectual Property Rights & Cheminformatics  
(Optional course-2)/ Research Methodology

## Scheme of Examination

The performance of the learners shall be evaluated into two parts. The learner's performance shall be assessed by Internal Assessment with 40% marks in the first part and by conducting the Semester End Examinations with 60% marks in the second part. The allocation of marks for the Internal Assessment and Semester End Examinations are as shown below-

### A) Internal Assessment: 40 % 40 Marks

Sr. No.	Particular	Marks
01	One periodical class test / online examination to be conducted in the given semester	20 Marks
02	One case study /review / project with presentation based on curriculum to be assessed by the teacher concerned	15 Marks
	Presentation	10 Marks
	Written Document	05 Marks
03	Active participation in routine class instructional deliveries and overall conduct as a responsible learner, mannerism and articulation and exhibit of leadership qualities in organizing related academic activities	05 Marks

## Question Paper Pattern

*(Periodical Class Test for the Courses at Post Graduate Programmes)*

Maximum Marks: 20

Duration: 40 Minutes

Questions to be set: 02

All Questions are Compulsory

Question No.	Particular	Marks
Q-1	Match the Column / Fill in the Blanks / Multiple Choice Questions/ Answer in One or Two Lines (Concept based Questions) ( 1 Marks / 2 Marks each)	10 Marks
Q-2	Answer in Brief (Attempt any Two of the Three) (5 Marks each)	10 Marks

### B) Semester End Examination: 60 % 60 Marks

- Duration: The examination shall be of  $2\frac{1}{2}$  hours duration.
- There shall be five questions each of 12 marks.

Question may be subdivided into sub-questions a, b, c... and the allocation of marks depends on the weightage of the unit.

## ***Question Paper Pattern for Semester End Examination***

<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.	
	1. There shall be five questions each of 12 marks. All questions are compulsory and will have internal options. Question may be subdivided into sub-questions a, b, c... and the allocation of marks depends on the weightage of the unit.	
	Q-1	From Unit – I (having internal options.) 12 M
	Q-2	From Unit – II (having internal options.) 12M
	Q-3	From Unit – III (having internal options.) 12M
	Q-4	From Unit – IV(having internal options.) 12M
Q-5	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>	Particulars of External Practical Examination	<b>Marks%</b>
1	Laboratory Work	80
2	Journal	10
3	Viva	10
	<b>TOTAL</b>	<b>100</b>

### **❖ Passing Standard**

The learners shall have to obtain a minimum of 40% marks in aggregate for each course where the course consists of Internal Assessment and Semester End Examination. The learners shall obtain minimum of 40% marks (i.e. 16 out of 40) in the Internal Assessment and 40% marks in Semester End Examination (i.e. 24 Out of 60) separately, to pass the course and minimum of grade D in each project wherever applicable to pass a particular semester.

### **❖ Guidelines and Evaluation pattern for project work (100 Marks)**

#### **Introduction**

Inclusion of project work in the course curriculum of the M.Sc. programme is one of the ambitious aspects in the programme structure. The main objective of inclusion of project work is to inculcate the element of research work challenging the potential of learner as regards to his/ her eager to enquire and ability to interpret particular aspect of the study in his/ her own words. It is expected that the guiding teacher should undertake the counselling sessions and make the awareness among

the learners about the methodology of formulation, preparation and evaluation pattern of the project work.

- There are two modes of preparation of project work
  1. Project work based on research methodology in the study area
  2. Project work based on internship in the study area

Choice Based Credit ,Grading and Semester System (CBCGS)  
To be implemented from the Academic year 2020-2021  
**M.Sc.-II Analytical Chemistry**  
**Semester- III**

Course Code	Unit	Topics	Credits	L / Week
<b>PSC3QAC</b>	I	Quality in Analytical Chemistry-I	4	1
	II	Quality in Analytical Chemistry-II		1
	III	Chromatographic Techniques-I		1
	IV	Chromatographic Techniques-II		1
<b>PSC3AIT</b>	I	Spectral Methods -I	4	1
	II	Spectral Methods -II		1
	III	Electroanalytical Methods		1
	IV	Miscellaneous Techniques		1
<b>PSC3BCF</b>	I	Bio-analytical Chemistry	4	1
	II	Immunological Methods		1
	III	Food analysis-I		1
	IV	Food analysis-II		1
<b>PSC3ENC</b>	I	Air Pollution	4	1
	II	Water Quality Standards		1
	III	Other Types of Pollution		1
	IV	Industrial Materials		1
<b>PSC3POA</b>	I	Pharmaceutical Analysis	4	1
	II	Drugs		1
	III	Forensic Analysis		1
	IV	Cosmetics Analysis		1
<b>PSC3QAP</b> <b>PSC3AIP</b> <b>PSC3BCP</b> <b>PSC3ENP/</b> <b>PSC3POP</b>	-	Practical Course	8	16

**Choice Based Credit ,Grading and Semester System (CBCGS)  
To be implemented from the Academic year 2020-2021  
M.Sc.-II Analytical Chemistry  
Semester- IV**

<b>Course Code</b>	<b>Unit</b>	<b>Topics</b>	<b>Credits</b>	<b>L / Week</b>
<b>PSC4QAC</b>	I	Separation Science	4	1
	II	Separation, Analysis and Standardization of Herbal based products		1
	III	Green Chemistry		1
	IV	Advanced Techniques		1
<b>PSC4AIT</b>	I	Spectral Methods -III	4	1
	II	Spectral Methods -IV		1
	III	Radiochemical and Thermal Methods		1
	IV	Hyphenated Techniques		1
<b>PSC4STA</b>	I	Effluent Treatment	4	1
	II	Solid Waste Management		1
	III	Plastics and Polymers		1
	IV	Metallurgy		1
<b>PSC4IPR</b>	I	Introduction to Intellectual Property Rights-I	4	1
	II	Introduction to Intellectual Property Rights-II		1
	III	Introduction to Chemoinformatics		1
	IV	Application of Chemoinformatics		1
<b>PSC4REM</b>	I	Resources	4	1
	II	Data Analysis		1
	III	Methods of Scientific Research and Writing		1
	IV	Chemical Safety and Ethical Handling of Chemicals		1
<b>PSC4QAP PSC4AIP PSC4STP</b>	-	Practical Course	8	16
<b>PSC4IPP/ PSC3REP</b>		Project Evaluation / Industrial Internship		

**Choice Based Credit, Grading and Semester System (CBCGS)**  
**(To be implemented from the Academic year 2020-2021)**

<b>M.Sc. ANALYTICAL CHEMISTRY SEMESTER – III</b>		
<b>PSC3QAC</b>		
<b>Quality in Analytical Chemistry</b>		
UNIT 1	Quality In Analytical Chemistry - I	
	<p>1.1 Sampling: Definition, types of sample, sampling plan, quality of sample, subsampling, Sampling of raw materials, intermediates and finished products. Sample preparations – dissolution technology and decomposition, storage of samples. Pre-treatment of samples: soil, food and cosmetics. (8L)</p> <p>1.2 Selection of the Method: sources of methods, factors to consider when selecting a method, performance criteria for methods used, reasons for incorrect analytical results, method validation, and quality by design (PAT).(7L)</p>	
UNIT II	Quality In Analytical Chemistry - II	15
	<p>2.1 Measurement of uncertainty: Definition and evaluation of uncertainty, putting uncertainty to use, interpretation of results and improving the quality of results. (4L)</p> <p>2.2 Signal to noise: Signal to noise ratio, sources of noise in instrumental analysis. Signal to noise enhancement, hardware devices for noise reduction, software methods for noise reduction. (6L)</p> <p>2.3 Pharmaceutical Legislation: introduction to drug acts, drug rules (schedules), concept of regulatory affairs in pharmaceuticals, review of GLP and GMP and their regulations for analytical labs, roles and responsibilities of personnel, appropriate design and placement of laboratory equipment, requirements for maintenance and calibration. (5L)</p>	
UNIT III	Chromatographic Techniques -I	15
	<p>3.1 Ion exchange chromatography: Ion exchange equilibria, breakthrough capacity, inorganic ion exchangers, synthetic ion exchangers, chelating resins and their applications for separation of inorganic and organic compounds. (8L)</p> <p>3.2 Ion chromatography: Principle, instrumentation with special reference to separation and suppressor columns, applications. (2L)</p> <p>3.3 Exclusion chromatography : Theory, instrumentation and applications of gel permeation chromatography, retention behavior, inorganic molecular sieves, determination of molecular weight of polymers, (5L)</p>	
UNIT IV	Chromatographic Techniques -II	15
	<p>4.1 Supercritical fluid Chromatography: Theory, concept of critical state of matter and supercritical state, types of supercritical fluids, instrumentation, applications to environmental, food, pharmaceuticals and polymeric analysis.</p>	



(8L)

4.2 Affinity Chromatography: principle, instrumentation and applications (4L)  
Optimum pressure liquid chromatography (OPLC) (3L)

**List of books and references:**

1. Quality in the analytical chemistry laboratory, E Prichard, John Wiley and sons N.Y 1997.
2. Quality assurance in analytical Chemistry, W Funk, V Dammann, G. Donnevert VCH Weinheim 1995.
3. Amit S. Patil *et. al.*, Quality by Design (QbD) : A new concept for development of Quality pharmaceuticals, International Journal of Pharmaceutical Quality Assurance; 4(2); 13-19.
4. Lalit Singh and Vijay Sharma, Quality by Design (QbD) Approach in Pharmaceuticals: Status, Challenges and Next Steps, Drug Delivery Letters, 2015, 5, 2-8. Quality in the analytical chemistry laboratory, E Prichard, John Wiley and sons N.Y 1997
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6. Chemical methods of separation, J A Dean, Van Nostrand Reinhold, 1969
7. Solvent extraction and ion exchange, J Marcus and A. S. Kertes Wiley INC 1969.
8. Analytical Chemistry, G. D. Christain, Wiley
9. Extraction Chromatography T. Braun, G. Ghersene, Elsevier Publications 1978.
10. Supercritical Fluid Extraction, Larry Taylor Wiley publishers N.Y. 1996
11. Ion exchange separation in analytical chemistry O Samuelson John Wiley 2<sup>nd</sup> ed 1963
12. Ion exchange chromatography Ed H.F Walton Howden, Hutchenson and Rossing 1976
13. Chromatographic and electrophoresis techniques I Smith Menemann Interscience 1960

**SEMESTER-III**  
**PSC3AIT**  
**Advance Instrumental Techniques**

UNIT I	Spectral Methods I	15
	<p>1.1 Surface Analytical Techniques: Preparation of the surface, difficulties involved in the surface analysis. (1L)  Principle, instrumentation and applications of Transmission Electron Microscopy (3L)</p> <p>1.2 Principle, instrumentation and applications of the following:  a. Secondary Ion mass spectroscopy. (4L)  b. Low-Energy Ion Scattering and Rutherford Backscattering (5L)  c. Atomic Emission Spectroscopy- electrical discharge sources (2L)</p>	
UNIT II	Spectral Methods – II	15
	<p>Principle, Instrumentation, and Applications of</p> <p>2.1 Electron Spin Resonance Spectroscopy (ESR) (5L)  2.2 Mossbauer's Spectroscopy (5L)  2.3 Particle-Induced X-Ray Emission (5L)</p>	
UNIT III	Electroanalytical Methods	15
	<p>Advanced Electroanalytical Techniques:-</p> <p>3.1 Current Sampled (TAST) Polarography, Normal and Differential Pulse Polarography (3L)  3.2 Potential Sweep methods- Linear Sweep Voltammetry and Cyclic voltammetry. (3L)  3.3 Potential Step method- Chronoamperometry (2L)  3.4 Controlled potential technique- Chronopotentiometry (2L)  3.5 Stripping Voltammetry- anodic, cathodic, and adsorption (2L)  3.6 Chemically and electrolytically modified electrodes and ultra-microelectrodes in voltammetry (3L)</p>	
UNIT IV	Miscellaneous Techniques	15
	<p>Principle, Instrumentation and Applications of:</p> <p>4.1 Chemiluminescence techniques (3L)  4.2 Chiroptical Methods : ORD, CD (5L)  4.3 Photoacoustic spectroscopy (3L)  4.4 Spectroelectrochemistry (4L)</p>	

### List of books and references:

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2. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West and F. J. Holler Holt-Saunders 6th Edition (1992)
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4. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A. Settle Jr 7<sup>th</sup> Ed CBS (1986)
5. Introduction to Instrumental Analysis, R. D. Braun, Mc Graw Hill (1987)
6. Electrochemical Methods, A. J. Bard and L.R. Faulkner, John Wiley, New York, (1980)
7. Electroanalytical Chemistry, J.J . Lingane, 2<sup>nd</sup> Ed Interscience, New York (1958)
8. Modern Polarographic Methods in Analytical Chemistry, A. M. Bond, Marcel Dekker, New York, 1980.
9. Electroanalytical Chemistry, Ed A. J. Bard and Marcel Dekker, New York, (A series of volumes)
10. Techniques and mechanism of electrochemistry, P. A. Christian and A. Hamnett, Blachie Academic and Professional (1994)
11. Wilson and Wilson's Comprehensive Analytical Chemistry, Ed. G. Svehla. (A series of Volumes)
12. Treatise on Analytical Chemistry, Eds. I. M. Kolthoff and Others, Interscience Pub. (A series of volumes).
13. Standard Methods of Chemical Analysis, Eds. F. J. Welcher, Robert E. Krieger Publishing Company, (A series of volumes)
14. Polarographic Methods in Analytical Chemistry, M. G. Arora, Anmol Publications Pvt Ltd
15. Surface Analysis –The Principal Techniques, 2<sup>nd</sup> Edition Edited by John C. Vickerman and Ian S. Gilmore 2009 John Wiley & Sons, Ltd. ISBN: 978-0-470-01763-0
16. NMR, NQR, EPR, and Mössbauer Spectroscopy in Inorganic Chemistry *R. V. Parish*. Ellis Horwood, Chichester

**SEMESTER – III**  
**PSCH3BCF**  
**Bioanalytical Chemistry and Food Analysis**

UNIT I	Bioanalytical chemistry	15
	1.1 Body Fluids 1.1.1 Composition of body fluids and detection of abnormal levels of glucose, creatinine, uric acid in blood, protein, ketone bodies and bilirubin in urine leading to diagnosis of diseases. (5L) 1.1.2 Physiological and nutritional significance of vitamins (water soluble and fat soluble) and minerals. (5L) 1.1.3 Analytical techniques (including microbiological techniques) for vitamins. (5L)	
UNIT II	Immunological Methods	15
	2.1 General processes of immune response, antigen-antibody reactions, precipitation reactions, radio, enzyme and fluoro-immuno assays.(8L)	
	2.2 Human Nutrition: Biological values and estimation of enzymes, carbohydrates, proteins, essential amino acids and lipids.(7L)	
UNIT III	Food Analysis - I	15
	3.1 Fuel value of food and importance of food nutrients (2L)	
	3.2 3.2.1 General idea about Food processing and preservation; 3.2.2 Food Additives: Legislation, Chemical preservatives, fortifying agents, emulsifiers, texturizing agents, flavours, colours, artificial sweeteners, enzymes. 3.2.3 Analysis of food for additives: Determination of SO <sub>2</sub> , nitrate and nitrites; determination of ascorbic acid; identification and determination of saccharine and identification of colors in food, natural colours (5L)	
	3.3 Food Contaminants– Trace metals and pesticide residues, contaminants from industrial wastes (polychlorinated biphenyls, dioxins), toxicants formed during food processing (aromatic hydrocarbons, nitrosamines), veterinary drug residues and melamine contaminants. (8L)	
UNIT IV	Food Analysis - II	15
	4.1 4.1.1 Food packaging – Introduction, types of packing materials, properties and industrial requirements.(2L) 4.1. 2 Processing and Quality requirements of Milk and milk products (cheese, butter and ice cream), vegetables and fruits, meat and meat products. (6L)	
	4.2. Analysis of Milk – Fat content, proteins, acidity, bacteriological quality and milk adulterants.(2L)	
	4.3 Analysis of Oils and Fats – acid value, sap value, iodine value. Determination of rancidity and antioxidants.(2L)	
	4.4 Analysis of spices (cloves, cinnamon, pepper, mustard) Determination of volatile oils and fixed oils.(3L)	

### **List of books and References:**

1. General, organic and biological chemistry, H. Stephen Stoker, Cengage Learning.
2. Advance dairy chemistry, vol 3, P. F. Fox, P. L. H. McSweeney Springer.
3. Physiological fluid dynamics vol 3, Nanjanagud Venkatanarayanasastri Chandrasekhara Swamy Narosa Pub. House, 1992
4. Molecular Biological and Immunological Techniques and Applications for food, edited by Bert Popping, Carmen Diaz-Amigo, Katrin Hoenicke, John Wiley & sons.
5. Food Analysis: Theory and practice, Yeshajahu Pomeranz, Clifton E. Meloan, Springer.
6. Principles of package development, Gribbin et al
7. Modern packaging Encyclopedia and planning guide, Macgra Wreyco.
8. Food Analysis, Edited by S. Suzanne Nielsen, Springer
9. Analytical Biochemistry, D, J. Homes and H. Peck, Longman (1983)
10. Bioanalytical Chemistry, S. R. Mikkelesen and E. Corton, John Wiley and sons 2004.
11. Analysis of food and beverages, George Charalanbous, Accademic press 1978.

## SEMESTER-III

### PSC3ENC

#### Environmental and Certain Industrially Important Matrials

UNIT I	Air Pollution	15
	<p>1.1 Sources, classification, pollutants and permissible limits.(2L)</p> <p>1.2 Sampling methods for air, flew gas ,Industrial Exhaust, stag samples etc. (2L)</p> <p>1.3 Importance of automobile exhaust control and its limits(2L)</p> <p>1.4 Sampling and analysis of: Particulate matter, aerosols, ammonia and organic vapors. (3L)</p> <p>1.5 Carbon credit and global issues related to air pollution.(3L)</p> <p>1.6 Greenhouse gases and their substitutes. (1L)</p> <p>1.7 Environmental Legislation: role of pollution control boards, article 48A and 51A, Motor Vehicle Act and method of analysis with respect to PUC. (2L)</p>	
UNIT II	Water Quality Standards	15
	<p>2.1 Water: quality and requirements of potable water, direct and indirect pollutants for potable water reservoirs, quality of potable water from natural sources. (6L)</p> <p>2.2 Bore well water quality and analytical parameters. Quality of bottled mineral water (3L)</p> <p>2.3 Process of purification of bore well water to bottled mineral water. (2L)</p> <p>2.4 Regulatory requirements for packaged drinking water (4L)</p>	
UNIT III	Other Types Of Pollution	15
	<p>3.1 Soil pollution and Soil Analysis : sources of soil pollution and their control, sampling of soil, determination of water holding capacity, determination total nitrogen, ammonia and nitrates, fertility of soil and effect of pollution on it, synthetic fertilizers and their long term effect on soil quality. (6L)</p> <p>3.2 Noise Pollution : sources, effects, methods of measurements and control measures.(2L)</p>	

	<p>3.3 Thermal Pollution: definition, source, impact, control measures, working of cooling towers and cooling ponds, involved economy. (3L)</p> <p>3.4 Radioactive pollutants: source, exposure hazards, precautions in handling and safety, Long term effects. (2L)</p> <p>3.5 Environmental Audits: concept of audit, authorities, evaluation methodology, benefits and certification (2L)</p>	
UNIT IV	Industrial Materials	15
	<p>4.1 Insecticides, Pesticides: definition, classification of insecticides pesticides. Biodegradation of insecticides and pesticides (5L).</p> <p>4.2 Soaps and Detergents: classification and composition, qualitative analysis, quantitative analysis of detergents- alkalinity, active ingredients and oxygen releasing capacity. Biodegradable detergents (5L)</p> <p>4.3 Petrochemical products: crude oils, fuels, and calorific values, fractional distillation process and fractions, properties of fuel, composition of fuel, flashpoint, fire point, corrosion test, carbon residue and impact on environment. (5L)</p>	

**List of Books and References:**

1. Environmental Chemistry, A. K. De, 2<sup>nd</sup> ED. Wiley (1989).
2. Environmental Pollution Analysis, S. M. Khopkar, John Wiely (1993).
3. Air Pollution Sampling And Analysis, Sharad Gokhale, IIT Guwahati, May 2009.
4. Environmental Pollution Analysis, S. M. Khopkar, New Age International publication (2011).
5. Water And Water Pollution (hand book) Ed., Seonard'l Ciacere, Vol I to IV, Marcel Dekker inc. N.York(1972)
6. Water pollution, Arvind kumar, APH publishing (2004)
7. Introduction to Potable Water Treatment Processes Simon Parsons, Bruce Jefferson, Paperback publication.
8. Guidelines for drinking-water quality, Third edition, (incorporating first and second addenda). WHO report.
9. Soil pollution, S.G. Misra and Dinesh Mani, APH Publishing Corporation, (2009).
10. Soil Pollution: origin, monitoring and remediation, Abraham Mirsal, Springer (2010).
11. Noise Pollution, Donald F Anthrop, Lexington Books, (1973)
12. Noise Effects Handbook: A Desk Reference to Health and Welfare Effects of Noise (1981) Available at NCL laboratories e- Library.

13. Chemistry, Emission Control, Radioactive Pollution and Indoor Air Quality Edited by Nicolas Mazzeo, InTech Publications (2011).
14. Environmental Protection Against Radioactive Pollution: N. Birsen, Kairat K. Kadyrzhanov, Springer publication , (2003).
15. Environmental law in India, Mohammad Naseem, Wolters Kluwer.
16. Environmental Protection, Law And Policy In *India* Kailash Thakur google books (1997).
17. Green chemistry An Introductory text, Mzike Lancaster, Royal Society of Chemistry (2002)
18. Pesticide Analysis Ed K. G. Das, Dekker (1981)
19. Analytical, Agricultural Chemistry S. L Chpra J.S Kanwar Kalyani publication
20. Soil and plant Analysis C.S Piper , Hans Publication



**SEMESTER – III**

**PSC3POA**

**Pharmaceutical and Organic Analysis**

UNIT I	Pharmaceutical Analysis	15
	<p>1.1 General idea regarding the Pharmaceutical Industry, definition and classification of drugs, introduction to pharmaceutical formulations and novel drug delivery system, classification of dosage forms. Role of FDA in pharmaceutical industries.(7L)</p> <p>Standardization and quality control of raw material and finished product Assay as per IP i) adrenaline, ii) Cephalexin, iii) ferrous fumarate, iv) paracetamol. (8L)</p>	
UNIT II	Drugs	15
	<p>2.1 Analysis of compounds based on functional groups, instrumental methods for analysis of drugs, proximate assays, assays of enzyme containing substances, biological and microbiological assays and tests. (8L)</p> <p>2.2 Limit tests, Sources of impurities and impurity profiling solubility tests, disintegration tests, stability studies, bioequivalence and bioavailability studies.(7L)</p>	
UNIT III	Forensic Science	15
	<p>3.1 Analytical Chemistry in Forensic Science: General idea.(2L)</p> <p>3.2 Forensic Analysis:                      3.2.1 Blood: Blood preservation blood stain analysis.)                      3.2.2 DNA profiling DNA typing procedures-RFLP, PCR, MVRPCR, Dot-blot, AMP-FLP, STR, other methods, paternity testing,                      3.2.3 Hair analysis: Structure and composition of hair, morphological examination, Chemical analysis of hair components and components remaining on or in hair.)                      3.2.4 Alcohol in body fluids: Sampling and sample preservation, analysis - GC, IR, enzymatic and other methods (5L)</p> <p>3.3 Analytical Toxicology: Isolation, identification and determination of:                      3.3.1 Narcotics: Heroin, morphine and cocaine.                      3.3.2 Stimulants: Amphetamines and caffeine.                      3.3.3 Depressants: Benzodiazepines, Barbiturates.                      3.3.4 Hallucinogens: LSD and Cannabis.                      3.3.5 Metabolites of drugs in blood and urine of addicts.                      3.3.6 Viscera, stomach wash, vomit and postmortem blood for poisons like – cyanide, arsenic, mercury, insecticides and pesticides. (8L)</p>	
UNIT IV	Cosmetic Analysis	15
	<p>4.1 Cosmetics: Introduction. Evaluation of cosmetic materials, raw materials and additives. Formulation, standards and methods of analysis.(2L)</p> <p>4.2 Deodorants and antiperspirants: Al, Boric acid, chlorides, sulphates, and methanamine. (3L)</p>	
	<p>4.3 Face powder: Ti, Fe, oxides of Ti, Fe and Al (total).(2L)</p>	

	4.4 Hair tonic: 2,5-diaminotoluene, potassium borates, sodium perborate, pyrogallol, resorcinol, salicylic acid, dithioglycollic acid (in permanent wavers)(4L)	
	4.5 Creams and Lotions: Types of emulsions, chloroform soluble materials, glycerol, pH emulsion, ash analysis, nonvolatile matter (IR spectroscopy) (3L)	
	4.6 Lipsticks: General analysis, lakes and fillers, trichloroethylene-acetone soluble contents.(1L)	

## References

- 1) Analytical Biochemistry, David J Holmes and Hazel Peck, Longman, 1983.
- 2) Bioanalytical Chemistry, Susan R Mikkelesen and Eduardo Cotton, John Wiley and Sons, 2004.
- 3) Analysis of food and beverages, George Charalanbous, Academic press, 1978.
- 4) Harry's Cosmetology, 7<sup>th</sup> Ed, Longman Scientific Co.
- 5) Formulation and Function of Cosmetics, Joseph Stefan Jellinek, Wiley Interscience, 1971.
- 6) Cosmetic Technology, Edward Sagarin, Interscience Publishers, 1957.
- 7) Modern Cosmetics, Edgar George Thommsen, Francis Chilson, Drug and Cosmetic Industry, 1947.
- 8) Encyclopedia of Industrial Chemical Analysis, Foster Dee Snell et al, Interscience Publishers, 1967.
- 9) Government of India Publications of Food, Drug and Cosmetic Act and Rules.
- 10) The Handbook of Drug Laws, M L Mehra, University Book Agency, Ahmedabad, 1997.
- 11) Chemical Analysis of Drugs, Takeru Higuchi, Interscience Publishers, 1995.
- 12) Text book of Pharmaceutical Analysis, Kenneth Antonio Connors, Wiley, 2001.
- 13) Food Processing and Preservation, B Sivasankar, Prentice - Hall of India Private Limited, 2007.
- 14) Food Additives, R M Pandey and S K Upadhyay, INTECH, Open Science/Open Minds.
- 15) Food Science, B Srilakshmi, New Age International (P) Ltd. Publishers, 2003.
- 16) Food Contaminants: Sources and Surveillance, Edited by C Creaser, R Purchase, Elsevier, 1991.
- 17) The Chemical Analysis of Food and Food Products, Morris B Jacobs.
- 18) FSSAI (Food Safety and Standards Authority of India) Manuals of Methods of Analysis of Foods (Oils and Fats, Milk and Milk Products, Food Additives), Ministry of Health and Family Welfare, Government of India.
- 19) Fundamentals of Urine and Body Fluid Analysis, Nancy A Brunzel, Elsevier health Sciences, 2013.
- 20) Lab Manual on Blood analysis and Medical Diagnostics, Dr Gayatri Prakash, S Chand and Company Ltd, New Delhi.
- 21) Manual of Medical Laboratory Techniques, S Ramakrishnan and K N Sulochana, Jaypee Brothers Medical Publishers (P) Ltd, 2012.

- 22) Indian Pharmacopeia, Volume I and II.
- 23) Forensic Chemistry, Suzanne Bell, Pearson Prentice Hall Publication, 2006.
- 24) Forensic Chemistry, David E Newton, Infobase Publishing, 2007.
- 25) Encyclopedia of Analytical Chemistry, Volume 3, Academic Press, 1995.
- 26) AOAC Volume I and II.

**SEMESTER-III PRACTICALS**  
**PSC3QAP**

1. Determination of the pK value of an indicator.
2. Determination of copper and bismuth in mixture by photometric titration.
3. Estimation of strong acid, weak acid and salt in the given mixture conductometrically.
4. Analysis of mixture of carbonate and bicarbonate (present in ppm range) using pHmetry.
5. Determination of copper by extractive photometry using diethyldithiocarbamate.

**PSC3AIP**

1. Estimation of drugs by non aqueous titration: Pyridoxine hydrochloride, Sulphamethoxazole.
2. Determination of percentage purity of methylene blue indicator.
3. Estimation of cholesterol and Uric acid in the given sample of blood serum
4. Estimation of fluoride in a tooth paste.
5. Determination of silica by molybdenum blue method.

**PSC3BCP**

1. Total reducing sugars before and after inversion in honey using: (a) Cole's Ferricyanide (b) Lane - Eynon method.
2. Analysis of lactose in milk
3. Estimation of Caffeine in tea
4. Estimation of Vitamin C in lemon Juice/squash by Dichlorophenol-indophenol method
5. Iodine value of oil / fat
6. Estimation of micronutrient from food by AAS (any two elements such as Fe, Cu, Zn, Mo, B, Mn)

**PSC3ENP/ PSC3POP**

1. To analyze Pyrolusite for: Fe by colorimetry and / or Mn by volumetry.
2. Analysis of Nicrome alloy for Ni (complexometry)
3. Analysis of Bauxite for Ti by colorimetry / Al by gravimetry / Fe (volumetry)
4. Analysis of water sample: Total hardness and salinity.
5. Analysis of water sample: Acidity and sulphate(Benzidine method).

**NOTE:**

1. The candidate is expected to submit a journal certified by the Head of the Department / institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he / she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily.
3. The list of the experiments performed by the candidate should be attached with such certificate.
4. Use of non-programmable calculator is allowed both at the theory and the practical examination.

**SEMSTER-IV****PSC4QAC****Quality In Analytical Chemistry**

UNIT I	Separation Science	15
	<p>1.1 Membrane separation processes: operating principles and applications of microfiltration, ultra-filtration, reverse osmosis, dialysis and electro-dialysis. (8L)</p> <p>1.2 Applications of Solvent extraction in Analytical Chemistry- recapitulation of solvent extraction, roles of solvent extraction in analytical chemistry, solvent extraction in sample preparation and pretreatment steps, solvent extraction as a means of analytical determination (7L)</p>	
UNIT II	Separation, Analysis and Standardization of Herbal based products.	15
	<p>2.1 Herbs as a raw material: Defination of herb, herbal medicine, herbal Medicinal products, herbal drug preparation. Sources of herbs. Selection, identification and authentication of herbal materials, drying and processing of herbal raw materials,drying and processing of herbal raw material.(6L)</p> <p>2.2Extraction of herbal materials: Choice of solvent for extraction, methods used for extraction and principles involved in extraction.(3L)</p> <p>2.3Standardization of herbal formulation and herbal extracts: Standardization of herbal extract as per WHO cGMP guidelines, Physical, Chemical,Spectral and toxillogical standardization,qualitative and quantitative esimations.(6L)</p>	

UNIT III	Green Chemistry	15
	<p>3.1 Principle and concepts of green chemistry: sustainable development and green chemistry, atom economy, examples of atom economic and atom uneconomic reactions, reducing toxicity (4L)</p> <p>3.2 Organic solvents: environmentally benign solutions, solvent free systems, supercritical fluids (only introduction) Ionic liquids as catalysts and solvents (4L)</p> <p>3.3 Emerging Green Technologies: photochemical reactions (advantages and challenges), examples. Chemistry using microwaves, sonochemistry and electrochemical synthesis. (4L)</p> <p>3.4 Designing Greener Processes: Inherently Safer Designs (ISD), Process intensification (PI) in-process monitoring. (3L)</p>	
UNIT IV	Advanced Techniques	15
	<p>4.1 Electrophoresis: introduction, factors affecting migration rate, supporting media (gel, paper, cellulose, acetate, starch, polyacrylamide, agarose, sephedax and thin layers) (2L)</p> <p>4.2 Techniques of Electrophoresis: low and high voltage, sds-page, continuous electrophoresis, capillary electrophoresis, zone, gel, isoelectric focusing, isotaechophoresis and miceller electro kinetic capillary chromatography, instrumentation, detection and applications. (8L)</p> <p>4.3 Introduction to Nanotechnology: One dimensional nano materials (nanofilms, nanolayers), two dimensional nanomaterials (nanotubes, nanowires), three dimensional nanomaterials (nanoparticles and quantum dots); consequences of the nanoscale, (morphology, electronic structure, optical properties), Applications of UV-Vis, IR and Raman, X-ray diffraction, SEM, TEM and XPS, probe analysis (AFM) in characterization of nanomaterials. (5L)</p>	

**List of Books and references:**

1. Research Methodology: Methods & Techniques by C R Kothari, 2e, Wishwa Publication, New Delhi
2. Research Methodology by D K Bhattacharyya, 1 e, Excel Books, New Delhi, 2003
3. How to Research by Loraine Blaxter, Christina Hughes and Molcolm Tight, Viva Books Pvt.Ltd., New Delhi
4. Chemical methods of separation, J A Dean, Van Nostrand Reinhold, 1969
5. Solvent extraction and ion exchange, J Marcus and A. S. Kertes Wiley INC 1969.
6. Extraction Chromatography, T. Braun, G. Ghersene, Elsevier Publications 1978.
7. Super critical fluid extraction, Larry Taylor Wiley publishers N.Y. 1996
8. Ion exchange separation in analytical chemistry, O Samuelson John Wiley 2nd ed 1963
9. Ion exchange chromatography, Ed H.F Walton Howden, Hutchenson and Rossing 1976
10. Chromatographic and electrophoresis techniques, I Smith Menemann Interscience 1960
11. Green chemistry and catalyst, R. A. Sheldon, Isabella Arends, Ulf Hanefeld Wiley VCH verlag GmbH & co.
12. Sustainable residential development: planning and design for green neighborhoods. Avi Friedman, McGraw Hill professional.

**SEMESTER-IV****PSC4AIT****Advanced Instrumental Techniques**

UNIT I	Spectral Methods III	15
	<p>NMR Spectroscopy</p> <p>1.1 Theory and Instrumentation- recapitulation, FTNMR, 2D NMR,- FID signal generation mechanism, Techniques in 2D NMR- homo nuclear correlation spectroscopy (COSY), total correlation spectroscopy (TOCSY), heteronuclear correlation (HETCOR) (9L)</p> <p>1.2 Radio waves in imaging- principle instrumentation and applications of MRI (3L)</p> <p>1.3 Application of NMR to other nuclei C<sup>13</sup>, P<sup>31</sup> and F<sup>19</sup> spectroscopy (3L)</p>	
UNIT-II	Spectral Methods IV	15
	<p>2.1 Mass spectrometry: recapitulation, correlation of mass spectra with molecular structure- interpretation of mass spectra, analytical information derived from mass spectra- molecular identification, metastable peaks, Fragmentation Reactions (9L)</p> <p>2.2 Raman spectroscopy: Principle Theory Instrumentation , techniques(SERS and Resonance Raman) and Applications of Raman spectroscopy (6L)</p>	
UNIT III	Radiochemical And Thermal Methods	15
	<p>3.1 Activation analysis- NAA ,radiometric titrations and radio-release methods(7L)</p> <p>3.2 Thermal analysis- Principle, Interfacing , instrumentation and Applications of</p> <p>(a) Simultaneous Thermal Analysis- TG-DTA and TG-DSC</p> <p>(b) Evolved gas analysis- TG-MS and TG-FTIR (8L)</p>	
UNIT IV	Hyphenated Techniques	15
	<p>4.1 concept of hyphenation, need for hyphenation, possible hyphenations. ( 2 L )</p> <p>4.2 Interfacing devices and applications of GC – MS, ICP -MS, GC - IR, Tandem Mass Spectrometry, LC – MS: HPLC-MS, CE-MS. (13L)</p>	



### List of Books and references:

1. Analytical Chemistry, G. D. Christian, 4<sup>th</sup> Ed. John Wiley, New York (1986)
2. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West and F. J. Holler Holt-Saunders 6<sup>th</sup> Edition (1998)
3. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann 5 Ed.
4. Instrumental methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A.
5. Thermal methods of Analysis, P. J. Haines, Blackie Academic & Professional, London (1995)
6. Thermal Analysis, 3<sup>rd</sup> Edition W. W. Wendlandt, John Wiley, N.Y. (1986)
7. Principles and Practices of X-ray spectrometric Analysis, 2 NY, (1975)
8. Ed E. P. Bertain, Plenum Press, Nuclear Analytical Chemistry, D. Bane, B. Forkman, B. Persson, Chartwell - Bratt Ltd (1984)
9. Standard Methods of Chemical Analysis, Eds. F. J. Welcher, Robert E. Krieger Publishing Company, A series of volumes
10. A Complete Introduction to Modern NMR Spectroscopy 1<sup>st</sup> Edition by Roger S. Macomber
11. Spectrometric Identification of Organic Compounds Hardcover – by Robert M. Silverstein Wiley
12. Tandem Techniques (Separation Science Series) 1<sup>st</sup> Edition by Raymond P. W. Scott John Wiley & Sons Ltd, 1997
13. Encyclopedia of Analytical Science, Editors-in-Chief: Paul Worsfold, Alan Townshend, and Colin Poole ISBN: 978-0-12-369397-6
14. Encyclopedia of Analytical Chemistry: Applications, Theory, and Instrumentation. Meyers Robert A Meyers
15. Introduction to Thermal Analysis Techniques and Applications Edited by Michael E. Brown
16. Principles and Applications of Thermal Analysis Edited by Paul Gabbott

**SEMESTER – IV**  
**PSC3STA**  
**Selected Topics in Analytical Chemistry**

UNIT I	Effluent Treatment	15
	1.1 Effluent treatment plant general construction and process flow charts(3L) 1.2 Treatment and disposal of Sewage.(3L) 1.3. Effluent parameters for metallurgical industry.(2L) 1.4 Permissible limits for metal (example Cr, As, Pb, Cd etc) traces in the effluent.(2L) 1.5 Recovery of metals from effluent, modern methods – Electrodialysis, Electrodeposition and Ion Exchange etc.(3L) 1.6 Recycle and reuse of process and treated (effluent) water(2L)	
UNIT – II	Solid Waste Management	15
	2.1 Solid waste management: objectives, concept of recycle, reuse and recovery (3L) 2.2 Methods of solid waste disposal.(2L) 2.3 Treatment and disposal of sludge / dry cake (3L) 2.4 Managing non-decomposable solid wastes(2L) 2.5 Bio- medical waste : Introduction , Classification and methods of disposal (5L)	
UNIT – III	Plastics and Polymers	15
	3.1 Classification of plastic, determination of additives, molecular weight distribution, analysis of plastic and polymers based on styrene, vinyl chloride, ethylene, acrylic and cellulosic plastics. (5L) 3.2 Metallic impurities in plastic and their determination, (2L) 3.3 Impact of plastic on environment as pollutant.(2L) 3.4 Paints and pigments: Types of paints pigments, determination of volatile and non - volatile components, Flash point (significance and method of determination), separation and analysis of pigments, binders and thinners.(3L) 3.5 Role of Organo silicones in paints and their impact on environment.(3L)	
UNIT – IV:	Metallurgy	15
	4.1 Ores and minerals: Dressing of ores, pollution due to metallurgical processes (ore dressing, calcination, smelting ) (3L) 4.2 Chemical analysis of ores for principal constituents : Galena, Pyrolusite, Bauxite, Hematite, Monazite (4L) 4.3 Alloys: definition, analysis of Cupronickel, Magnesium, Steel And Stainless Steel, Bronze, Gun metal.(4L) 4.4 Techniques of purification: Zone refining, analysis of high purity materials like silicon , vacuum fusion and extraction techniques. (4L)	

**List of Books and References:**

1. Environmental Pollution Analysis, S. M. khopkar, New Age International publication (2011).
2. Water and water pollution (hand book) Ed., Seonard'1 Ciacere, Vol I to IV, Marcel Dekker inc. N.Y.(1972)
3. Water pollution, Arvind kumar, APH publishing (2004)
4. Introduction to Potable Water Treatment Processes Simon Parsons, Bruce Jefferson, Paperback publication.
5. Solid waste management, K Sasikumar and Sanoop Gopi Krishna PHI publication (2009)
6. Solid waste management, Surendrakumar Northen Book Center (2009)  
i. rd
7. Handbook of chemical technology and pollution control 3 Edn Martin Hocking AP Publication (2005).
8. 8 Fundamental Concepts of Environmental Chemistry, Second Edition G. S. Sodhi , Alpha Science, 2005
9. Chemical analysis of metals ; Sampling and analysis of metal bearing ores: American Society for Testing and Materials 1980 - Technology & Engineering
10. Manual of Procedures for Chemical and Instrumental Analysis of Ores, Minerals, and Ore Dressing Products. Government of India Ministry of Steel & Mines, Indian Bureau of Mines, 1979.
11. Alloying: understanding the basics, edited by Joseph R. Davis, ASM International (2001).
12. Zone refining and allied techniques, Norman L. Parr, G. Newnes Technology & Engineering (1960).

**SEMESTER – IV****PSC4IPR****Intellectual Property Rights & Cheminformatics**

UNIT I	Introduction to Intellectual Property-I	15
	<p>1.1 : Historical Perspective, Different types of IP, Importance of protecting IP.(2L)</p> <p>1.2: Patents: Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India (5L)</p> <p>1.3: Industrial Designs: Definition, How to obtain, features, International design registration.(2L)</p> <p>1.4: Industrial Designs: Definition, How to obtain, features, International design registration.(2L)</p> <p>1.5: Trade Marks: Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc. (2L)</p> <p>1.6: Geographical Indications: Definition, rules for registration, prevention of illegal exploitation, importance to India. (2L)</p>	
UNIT – II	Introduction to Intellectual Property-II	15
	<p>2.1 Trade Secrets: Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.[2L]</p> <p>2.2 IP Infringement issue and enforcement: Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. [2L]</p> <p>2.3 Economic Value of Intellectual Property: Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer. [5L]</p> <p>2.4 Different International agreements: (a) World Trade Organization (WTO): [5L] (i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement (ii) General Agreement on Trade Related Services (GATS); Madrid Protocol. (iii) Berne Convention (iv) Budapest Treaty (b) Paris Convention [6L] WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity</p>	
UNIT – III	Introduction to Chemoinformatics	15
	<p>3.1 History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.[5L]</p> <p>3.2 Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification. [5L]</p> <p>3.3 Searching Chemical Structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods,</p>	

	basics of computation of physical and chemical data and structure descriptors, data visualization. [5L]	
UNIT – IV	Applications of Chemoinformatics	15
	Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target, Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand based and Structure based Drug design, Application of Cheminformatics in Drug Design.	

**SEMESTER – IV**  
**PSC4REM**  
**Research Methodology**

UNIT I	Resources	15
	<p>1.1 Print: Primary, Secondary and Tertiary sources.</p> <p>1.2 Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents,</p> <p>1.3 Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.[5L].</p> <p>1.4 Digital: Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books,</p> <p>Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus. [5L]</p> <p>Information Technology and Library Resources: Internet and World wide web, Internet resources for Chemistry, finding and citing published information. [5L]</p>	
UNIT – II	Data Analysis	15
	<p>2.1 The Investigative Approach: Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.</p> <p>2.2 Analysis and Presentation of Data: Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis.</p>	
UNIT – III	Methods of Scientific Research and Writing	15
	<p>3.1 Scientific papers: Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.</p> <p>3.2 Writing Scientific Papers: Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.</p>	
UNIT – IV	Chemical Safety & Ethical Handling of Chemicals	15
	<p>Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressure, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals..</p>	

## **PRACTICALS**

### **PSC4QAP**

1. Determination of pK value of H<sub>3</sub>PO<sub>4</sub> potentiometrically
2. Estimation of Na<sup>+</sup> in dairy whitener by flame photometry
3. Spectrophotometric determination of pH of buffer solution.
4. Simultaneous determination of Ti<sup>3+</sup> and V<sup>5+</sup> spectrophotometrically by H<sub>2</sub>O<sub>2</sub> method
5. To analyze Bronze for Zn by complexometric method

### **PSC4AIP**

1. Analysis of Aspirin/paracetamol as per IP with respect to identification, ash and assay
2. Analysis of detergents: Active detergent matter, alkalinity and Oxygen releasing capacity
3. Determination of the purity of crystal violet
4. Estimation of Ca in Ca-pentathionate/calcium lactate tablets
5. Canned food: Limits test for tin/zinc

### **PSC4STP**

1. Analysis of Calcium, Iron and phosphorous in milk.
2. Determination of SAP value of oil.
3. Estimation of Aldehyde in lemon grass oil / Cinnamon oil
4. Estimation of Glucose by Folin-Wu method
5. Analysis of water sample : Mn<sup>2+</sup> by colorimetric method

### **PSC4IPP/PSC4REP**

Project Evaluation/ Industrial Internship

**NOTE:**

1. The candidate is expected to submit a journal certified by the Head of the Department / institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he / she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.