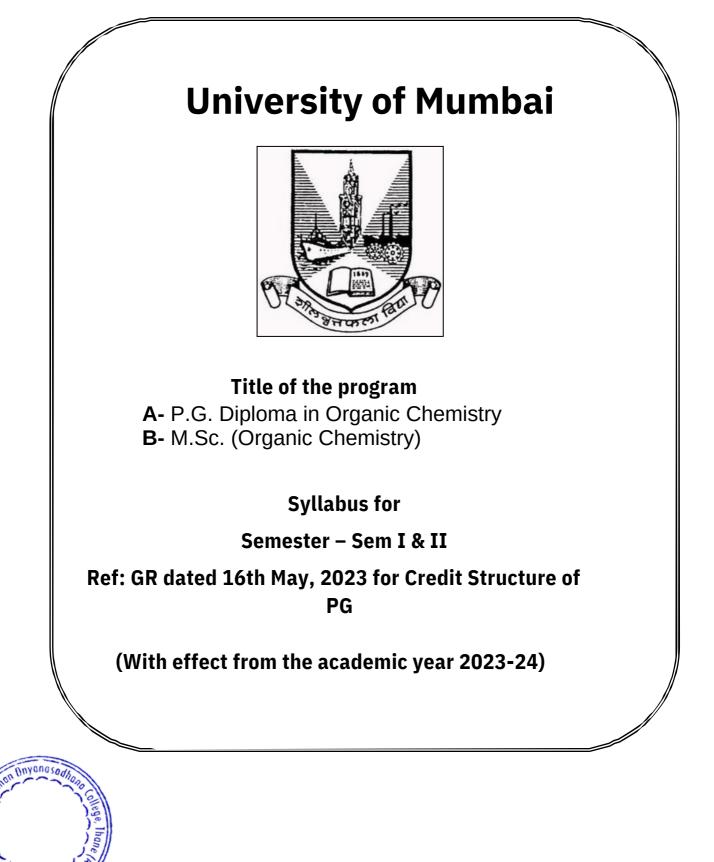
AC – Item No. –

# As Per NEP 2020



40) 8 83V

# University of Mumbai



(As per NEP 2020)

Sr. No	Heading		Particulars
	Title of program A	Α	<b>Title of the program</b> P.G. Diploma in Organic Chemistry
1	Title of program B	В	M.Sc. (Organic Chemistry)
	Eligibility (Program A)	A	B.Sc. Chemistry or equivalent qualification from other universities as may have been allowed by the relevant ordinances of this university
2	Eligibility (Program B)	в	B.Sc. Chemistry or equivalent qualification from other universities as may have been allowed by the relevant ordinances of this university
3	Duration of program	Tw	o Year
4	Intake Capacity	20	(variable as per college intake capacity)
5	Scheme of Examination		% Internal % External, Semester-End Examination
6	Standards of Passing	40	%
7	Semesters	A B	Sem I & II Sem I, II, III& IV
8	Program Academic Level	A B	6.0 6.0 & 6.5



9	Pattern	Semester
10	Status	New
11	To be implemented from Academic Year	From Academic Year: 2023-24

Sign of HOD

**Prof. Shivram S. Garje** Head of Department, Department of Chemistry, University of Mumbai



Sign of Dean,

**Prof. Shivram S. Garje** Dean, Science and Technology University of Mumbai



# Preamble

#### 1) Introduction

This program is designed to provide a comprehensive and in-depth understanding of

the fascinating world of Organic chemistry. Through a rigorous academic

curriculum and hands-on research experience, we aim to nurture the intellectual

curiosity and scientific acumen of our students, preparing them for successful careers in various sectors of the chemical sciences. The M.Sc. (Organic Chemistry)

course is structured to equip students with a strong theoretical foundation, practical

skills, and critical thinking abilities necessary to address the challenges and

opportunities in the diverse fields of chemistry. Our esteemed faculty members are

experts in their respective fields, with a passion for both teaching and research.

They are committed to providing a nurturing learning environment, encouraging

open discussions, and fostering collaborative research endeavors. Through their

mentorship, students will have the opportunity to engage in cutting-edge research

2) Any and Objectives of M.Sc. (Organic Chemistry) course are designed to the aims and objectives of M.Sc. (Organic Chemistry) course are designed to atoxideestudents with a well-itean selected advanced style ation in the field shic Onsenistry) poistor at have a selected by several selection in the field shic onderstanding of shape is to caterious research and any styles and represented in the selection of the

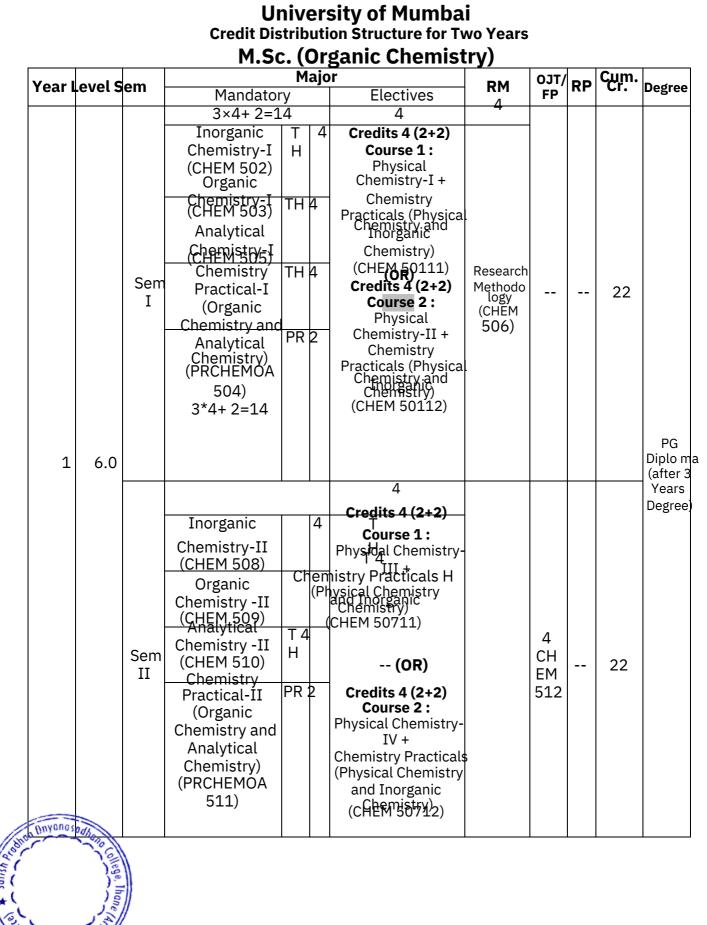
#### 3) Learning Outcomes

The learning outcomes of an M.Sc. (Organic Chemistry) course are designed to equip students with a comprehensive and advanced understanding of the field of chemistry. These learning outcomes reflect the knowledge, skills, and competencies that students are expected to gain upon successful completion of the program.

# 4) Any other point (if any)

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Credit Structure of the M.Sc. (Organic Chemistry) (Sem I, II, III & IV) (Table as per



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Cum. Cr. For	28	8	4	4		44	
PG Diploma							
E	xit Option: PG Diploma	(44 credits) after T	hree Year	UG D	egre	ee	

Year	Level		Major		RM	OJT/FP	RP		Degree
		(2yr)	3*4+ 2=14 Paper –I (Theoretical TH organic chemistry-I) (CHEM 641)	4 Paper IV (Medicinal Chemistry) + Practical (CHEM 64511)	-	-	4 (CHEM 646)	<b>Cr.</b> 22	
2	6.5	Sem III	Paper II (Synthetic TH Organic Chemistry- (CHEM 642) Paper III (Natural TH products and Spectroscopy-I) (CHEM 643) Organic Chemistry PR Practical (CHEM 644)	OR Paper IV (Biogenesis and green chemistry) + Practical (CHEM 64511) Advanced Topics in Organic Chemistry-I (CHEM 64513)					PG Degree after 3- yr UG Pr PG Degree yr UG
		Sem IV	3*4=12 Paper I (Theoretical TH 4 F organic chemistryotoclucts (CHEM 647) heterocyo chemistry (CHEM 650 Paper II (Synthetic Paper III (Bio Organic PR 4 (CHEM 648)	and clic /-II) 211)	-	-	6 (CHEM 651)	22	
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*	(mo) & ann	) and		1	1			6	

PG Degree							
Cum. Cr. For 2 Yr	54	16	4	4	10	88	
PG Degree							

#### Sign of HOD

**Prof. Shivram S. Garje** Head of Department, Department of Chemistry, University of Mumbai

HEAD DEPARTMENT OF CHEMISTRY UNIVERSITY OF MUMBAI Sign of Dean,

**Prof. Shivram S. Garje** Dean, Science and Technology University of Mumbai



Syllabus M.Sc. (Organic Chemistry) (Sem. I & II)



# <u>UNIVERSITY OF MUMBAI</u> Syllabus for M.Sc. (Organic Chemistry) Semester I and II **Choice-Based Credit System** Under New Education Policy (NEP) 2020 (To be implemented from the academic year, 2023-2024) **PROGRAM OUTLINE**

YEAR		COUI COI		COURSE TITLE	CREDITS	Page Number
	Mandatory Course-I	CHEM	502	Inorganic Chemistry-I	04	11
	Mandatory Course-II	CHEM	503	Organic Chemistry-I	04	16
	Mandatory Course-III	CHEM	505	Analytical Chemistry-I	04	20
M.Sc.	Mandatory Course Practical	PRCHEN 504	МОА	Chemistry Practical-I (Organic and Analytical Chemistry)	9 02	25
Sem- I	Elective 1	CHEM 50111		Physical Chemistry-I and Chemistry Practical (Physical and Inorganic Chemistry)	04	27
	Elective 2	CHEM 50112		Physical Chemistry-II and Chemistry Practical (Physical and Inorganic Chemistry)	04	33
	RM	CHEM	506	Research Methodology	04	39
	Mandatory Course-I	CHEM 5	08	Inorganic Chemistry-I	04	41
	Mandatory Course-II	CHEM 5	09	Organic Chemistry-II	04	45
	Mandatory Course-III	CHEM 5	510	Analytical Chemistry-I	: 04	49
M.Sc. Sem-II	Mandatory Course Practical	PRCHEN 511	MOA	Chemistry Practical-II (Organic and Analytical Chemistry)	02	53
	Elective 1	CHEM 50711		andysical Chemistry-III Chemistry Practical (Physical and Inorganic Chemistry)	04	55
	Elective 2	CHEM 50712		Physical Chemistry) Physical Chemistry-IV and Chemistry Practical (Physical and Inorganic	04	61



		Chemistry)		
OJT/FP	CHEM 512	Industrial Training/Field Project	9 04	67
		Proposed Examination Pattern		68

# **PROGRAMME SPECIFIC OUTCOME (PSOs)**

- **1.** Gain knowledge of the advanced concepts in the branch of chemistry, scrutinize and accomplish a solution to problems encountered in the field of research and analysis.
- 2. Apply the basic knowledge of chemistry to perform various tasks assigned to them at the workplace in industry and academia to meet the global standards.
- 3. **Declarized** ualitative and quantitative information of compounds using advanced spectroscopic methods which can further be analysed using practical skills inculcated in them during the course.
- **4.** Imbibe the attitude as well as aptitude of a scientific approach along with analytical reasoning with respect to the novel techniques actually implemented in the Industry.
- 5. Use the subject knowledge, communication and ICT skills to become an effective team leader/team member in the interdisciplinary fields.
- 6. Understand, Manage and contribute to solve basic societal issues and environmental concerns ethically based on principles of scientific knowledge gained.
- 7. Exhibit professional work ethics and norms of scientific development.



PROGRAM(s): M.ScI		SEMESTER: I						
Course: Pape	er-I	Course Code Course Title	-	5 <b>02)</b> ic Chemistry-I				
Teaching Scl	heme				Evaluation Scheme			
Lectures (Hours per week)	Practical (Hours per week)	Hours per(Hours perCreditAssessment(CA)						
04	NA	-	04	50	50			

# Learning Objectives:

## **Inorganic Chemistry**

- 1.To develop the ability to correlate fundamental theories of spatial orientations of molecules based on wave mechanics with advancedconceptsin chemical bonding ,symmetry of molecular systems and Structural aspects of inorganic solids.
- 2. To gain theoretical knowledge of cutting edge topics such as solid state lasers and contemporary Methods of preparation of nanomaterial's .
- 3.To learn about diverse tools available for characterization of coordination compounds in order to enhance competency while applying for practical purpose

# Course Outcomes:

- 1. The learner will know the important fundamental concept of Group Theory, which helps them in understanding the properties and bonding in polyatomic molecules.
- 2. The learner get the knowledge about the various techniques used for Characterization coordination compounds.
- 3. The learners develops the skill in interpretation of the spectra.

4. Thelearnerswill get comprehensive idea about established instrumental techniques and Significant characterization tools available to study inorganic complexes having wide applications in industries.



#### Course Code : (CHEM 502) Course Title:-Inorganic Chemistry-I

#### Unit – I

## Unit I Chemical Bonding: [15 L]

1.1 Recapitulation of hybridization Derivation of wave functions for sp, sp2, sp3 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 diatomic species of First transition Series.

1.4 Molecular Orbital Theory for Polyatomic species considering  $\boldsymbol{\sigma}$  bonding for

SF6,

CO2, B2H6, I3 - molecular species.

1.5 Weak forces of attraction: Hydrogen bonding - concept, types, properties,

methods

of detection and importance. Van der Waal's forces, ion-dipole, dipole-dipole, 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. a) Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations. The Great Orthogonality Theorem and application in construction of character tables for point groups C2v, C3v and C2h, structure of character tables.

b) Determination of symmetry species for translations and rotations.

c) Mulliken"s notations for irreducible representations.

d) Reduction of reducible representations using reduction formula.

2.4. Applications of Group Theory Symmetry adapted linear combinations (SALC),



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)], AB2

[fluorite

(CaF2) and anti-fluorite structures, rutile (TiO2)

3.1.3. Solid state lasers: Introduction, Types, Working & Applications

3.2 Nanomaterials-

3.2.1 Preparative methods, Chemical methods, solvothermal, combustion

synthesis,

microwave, coprecipitation, Langmuir-Blodgett(LB) method, biological methods, synthesis using microorganism.

3.2.2 Applications in the field of semiconductors, solar cells. Unit  ${\bf IV}$ 

Characterization of Coordination compounds [15L] 4.1. Methods of

Characterization: thermal studies, Conductivity measurements,

electronic spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods.

4.2. Introduction to Orgel& Tanabe Sugano Diagram, Terms, Splitting of terms in Octahedral, weak field, Calculation of electron parameters  $\Delta$ ,  $\beta$ , C and ratio with suitable examples.

4.3. Determination of formation constants of metal complexes (Overall and

Stepwise):

Comparative studies of Potentiometric and spectrophotometric 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.

7. Peter Atkins and Julio de Paula, Atkin"s*Physical Chemistry*, 7th Edn., Oxford University Press, 2002.

8. An introduction to Lasers Theory and Applications by M.N. Avadhanulu,P.S.Hemne, S.Chand publication.

9. Advances in solid state lasers development and Applications by M. Grishin

10. Solid state Lasers- A Graduate Text by Walter Koechner, Michael Bass, Springer.

11. Rare earth materials-properties & applications by A.R. Jha, CRC Press

**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).



PROGRAM(s): M.ScI Course: Paper-II		SEMESTER: I Course Code: <b>( CHEM 503)</b> Course Title:- Organic Chemistry-I					
Lectures (Hours (CA) per week) Practical (Hours per per week)		Tutorial (Hours per week)	Credit	Continuous Assessment (Marks- 50)	Semester End Examination (Marks- 50)		
04	NA	-	04	50	50		
concepts in reaction Mechanism, stereochemistry, different reactions and reagents. 2. To apply the basic knowledge of Organic chemistry to perform various tasks assigned at the workplace in industry and academia to meet the job requirements as per global st 3. Accomplish a solution to problems encountered in the field of research. Course Outcomes:							
	leting the cou	rse students	will be ab	le to:			
After comp	-			le to: from its structure	9.		
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After comp 1) predict 2) unders Mecha 3) unders	t the reactivity stand different anism	of organic co methods use amental cono	ompound f ed for dete cept in ste	from its structure	ganic Reaction		
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#### Course Code : (CHEM 503) Course Title:-Organic Chemistry-I

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

- **1.Ihermodynamic 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.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 pKa values, Leveling effect and non-aqueous solvents. Acid and base catalysis general and specific catalysis with examples.

# Unit-II

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# Stereochemistry: (15 L)

- **2.1. Concept of Chirality:** Recognition of symmetry elements.
- **2.2. Molecules with tri- and tetra-coordinate centers**: Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities.

**2.3. Molecules with two or more chiral centers:** Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Interconversion of **Eisostatitu Sendlor**se, Newman and Flying wedge projections.

symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereogenic, chirotopic, and pseudoasymmetriccentres. R-S nomenclature for chiral centres in acyclic and cyclic compounds.

**2.4. 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.

2.5. Prochirality: Chiral and prochiralcentres; 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 prochiralcentres ii) a chiral as well as a prochiralcentre, iii) a prochiral axis iv) a prochiral plane v) pro-pseudoasymmetriccentre. Symbols for enantiotopic and diastereotopic face.

# Unit III

# Nucleophilic substitution reactions and Aromaticity (15L)

## **3.1. Nucleophilic substitution reactions: (9 L)**

- 3.1.1 Aliphatic nucleophilic substitution: \$N1, SN2, SNreactions, mixed SN1 and SN2 and SET mechanisms. SN reactions involving NGP participation by aryl rings, σ and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. SNcA, S<sup>1</sup> and S N2<sup>°</sup> reactions. SN at sp (vinylic) carbon.
- **3.1.2 Aromatic nucleophilic substitution:** SNAr, SN1, benzyne mechanisms. Ipso, cine, tele and vicarious substitution.
- **3.1.3 Ester hydrolysis:** Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.

# 3.2. Aromaticity: (6 L)

3.2.1. Huckel's (4n+2) and 4n rules, structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.

3.2.2. Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene (C60).

#### Unit-IV

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

- **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 K2Cr2O7/H2SO4 (Jones reagent), CrO3-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 HIO4; cycloalkanones using CrO3; carbon-carbon double bond using ozone, KMnO4, CrO3, NaIO4 and OsO4; aromatic rings using RuO4 and NaIO4.

**4.1.4. Oxidation involving replacement of hydrogen by oxygen:** oxidation of CH2 to CO by SeO2, oxidation of arylmethanes by CrO2Cl2 (Etard oxidation).

acid Raeyer-Villiger oxidation)

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

- **4.2.1. Reduction of CO to CH2 in aldehydes and ketones-**Clemmensen reduction, Wolff-Kishner reduction and Huang-Minlon modification.
- **4.2.2. Metal hydride reduction:** Boron reagents (NaBH4, NaCNBH3, diborane, 9-BBN, Na(OAc)3BH, aluminium reagents (LiAlH4, DIBAL-H, Red Al, L and K- selectrides).
- **4.2.3.** N2H2 (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 NH3 mediated reduction of aromatic compounds (Birch reduction) and Alkynes.

#### **Reference Books**.

www gauge gow

- 1. Physical Organic Chemistry, NeilIsaacs
- 2. Modern Physical Organic Chemistry, Eric V. Anslynand Dennis A.Dougherty
- 3. Comprehensive Organic chemistry, Barton and Ollis, Vol1
- 4. Organic Chemistry, J. Claydens, N. Greeves, S.Warren and P. Wothers, Oxford University Press.
- 5. Advanced Organic Chemistry, F.A. Careyand R.J. Sundberg, Part A and B, Plenum Press.
- 6. Stereochemistry: Conformation and mechamism, P.S. Kalsi, New Age International, New Delhi.
- 7. Stereochemistry of carbon compounds, E.L Eliel, S.H Wilen and L.N Manden, Wiley.
- Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. New International Publishers Ltd. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
- 10. Advanced Organic Chemistry: Reactions and mechanism, B. Millerand R.Prasad, Pearson Education.
- 11. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, AcademicPress.
- 12. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
- 13. Writing Reaction Mechanism inorganic chemistry, A.Miller, P.H.Solomons, Academic Press.
- 14. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
- 15. Mechanism in Organic Chemistry, Peter sykes, 6th edition onwards.
- 16. Modern Methods of Organic Synthesis, W. Carruthers and Iain Coldham, Cambridge University Press.
- 17. Organic Synthesis, Jagdamba Singh, L. D. S. Yadav, Pragati Prakashan.
- Weiversity Press.
  - 19. Organic reactions and their Mechanisms, P.S. Kalsi, New Age International Publishers.
  - 20. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Nelson Thornes

PROGRAM(s)	: M.ScI	SEMESTER	:I					
Course: Pape	er-III	Course Code: <b>( CHEM 505)</b> Course Title:- Analytical Chemistry-I						
Teaching Sch	ieme				Evaluation Scheme			
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)			
04	04 NA <sup>-</sup> 04 50 50							
Learning Obje 1. To enable l		e comprehe	nsive kno	wledge, understa	anding of the types			

1. To enable learners to have comprehensive knowledge, understanding of the types of instruments with operations and automated methods of analysis.

2. To apply the basic knowledge of quality systems, quality audit and quality managements,.

3. To enable learners to perform various tasks assigned to them at the workplace in industry and academia to meet the job requirements as per global standards.

4. To provide solutions to problems encountered in the field of analysis and research.

#### Course Outcomes:

After completion of this Course, the learner will be able to:

1. Understand various terms used in analytical chemistry.

2. Identify the different types of errors in analysis.

3. Sketch out the role and importance of total quality management, safety, accreditations and GLP in industries.

4. Understand the efficacy of automation in chemical analysis.

5. Design and specify applications of advanced analytical techniques in various fields.

6.Explore the applications of IR spectroscopy and thermal methods.

7. Perform basic calculations required in chemical analysis

8. Interpret the experimental results of analytical techniques. transformation reaction.



#### Course Code : (CHEM 505) Course Title:- Analytical Chemistry-I

#### Unit - I

#### 1.1 Language of Analytical Chemistry [8 L] 1.1.1 Analytical perspective [3 L]

Analytical approach.common analytical problems. Terms involved in analytical chemistry - Analysis, Analyte, Matrix, Determination, Measurement, Techniques, Methods, Procedures and protocol.

# 1.1.2 An overview of analytical methods [3 L]

Analytical methods - Types, classification and selection. Quantitative method of Analysis- Calibration method, Method of Standard addition, Internal standard method. Performance Characteristics of analytical method- Accuracy, Precision, Selectivity, Sensitivity, Detection limit (LOD,LOQ,LOL), Dynamic range and Robustness and Ruggedness.

# 1.1.3 Errors [2 L]

Types of errors. Absolute error, Relative error, Constant error and Proportionate errors. Minimization of errors.

# 1.2 Quality in Analytical Chemistry [7L]

# 1.2.1 Total Quality Management- TQM [3L]

Definition, Principles, Importance and benefits. Philosophy of implementation of TQM -Process steps, Advantages and Limitations i) Kaizen -Six steps ii) Six Sigma approach iii) 5S and 5S audit check for laboratories.

# **1.2.2** Safety in laboratories [2L]

Basic concept of safety in laboratory- The Industrial Hygiene Principles.Personal protection equipment (PPE).Occupational Safety and Health Administration (OSHA).

# 1.2.3 Accreditations [2L]

Accreditation of laboratories, NABL, Indian Government standards (ISI, HALLMARK, AGMARK).- Meaning and significance.

# Unit- II

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# 2.1 Calculations based on Chemical Principles [15 L]

(The following topics are to be covered in the form of numerical problems only)

- **2.1.1** Concentration of a solution based on volume and mass units.
- **2.1.2** Calculations of ppm, ppb and dilution of the solutions, concept of mmol.
- **2.1.3** Stoichiometry of chemical reactions, concept of kg /mol, limiting reactant, theoretical and practical yield.
- **2.1.4** Solubility and solubility equilibria, effect of presence of common ion in solution.
- **2.1.5** Calculations of pH of acids, bases, acidic and basic buffers.
- **2.1.6** Concept of formation constants, stability and instability constants, stepwise formation constants.

**2.1.7** 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 an oxidizing / reducing agent and its relationship with molarity).

## Unit III -Optical Methods [15 L]

#### 3.1 Infrared Absorption Spectroscopy [6 L]

- **3.1.1** Instrumentation: Sources, Sample handling, Transducers, Dispersive, nondispersive instrument.
- **3.1.2** Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on "Finger print" and Quantitative analysis.
- **3.1.3** Advantages and Limitations of IR.

#### 3.2 FT Technique [3 L]

- 3.2.1 Introduction of Fourier Transform.
- **3.2.2** Laser as a source of radiation, sample containers.
- **3.2.3** Detectors, Fiber optics.
- **3.2.4** FTIR and its advantages.

#### 3.3 Molecular Ultraviolet and Visible Spectroscopy [6 L]

3.3.1 Factors affecting molecular absorption: pH, temperature, solvent and effect of

substituents, types of transitions [emphasis on charge transfer absorption].

- **3.3.2** Applications of Ultraviolet and Visible spectroscopy:
  - i) On charge transfer absorption
  - ii) Simultaneous spectroscopy
  - iii) Derivative Spectroscopy

3.3.3 Dual spectrometry – Introduction, Principle, Instrumentation and Applications.

# Unit - IV Instrumental methods-I [15L]

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

- **4.1.1** Introduction: Types of thermal methods, comparison between TGA and DTA.
- **4.1.2** Differential Scanning Calorimetry-Principle, comparison of DTA and DSC.
- **4.1.3** Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting DSC Curves.
- **4.1.4** Applications Heat of reaction, Safety screening, Polymers, liquid crystals, Drug analysis.

#### 4.2 Automation in chemical analysis: [6 L]

- **4.2.1** Need for automation, Objectives of automation.
- **4.2.2** An overview of automated instruments.
- 4.2.3 Process control analysis, flow injection analysis, discrete automated systems,

automatic analysis based on multi-layered films, gas monitoring equipments.

**2.4** Automatic titrators.

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# References

Unit I

- 1. Modern Analytical Chemistry ; David Harvey, McGraw-Hill,Higher Education,(2000)
- 2. Principles of Instrumental Analysis ; Skoog, Holler and Nieman, 5th Edition, Ch: 1
- 3. Fundamentals of Analytical Chemistry, Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, 2004, Ch: 5.
- 4. Undergraduate Instrumental Analysis ; J W Robinson, Marcel Dekker, 6th edition Ch:1.
- 5. ISO 9000 Quality Systems Handbook; David Hoyle. 4th edition (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. 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. "A systematic approach for evaluating the quality of experimental toxicological and eco-toxicological data".;Klimisch, HJ; Andreae, M; Tillmann, U (1997). doi:10.1006/rtph.1996.1076. PMID 9056496.

# Unit II

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



# Unit III

1.

Principles of Instrumental Analysis, ; D. A. Skoog, F. J. Holler, T. A. Nieman, 5th Edition, Harcourt Asia Publisher. Chapter 6, 7,8, 13, 14, 16,17

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

# Unit IV

- 1. Introduction to instrumental methods of analysis; Robert D. Braun, Mc. Graw Hill (1987): Chapter 27,28
- 2. Thermal Analysis-theory and applications; R. T. Sane, Ghadge, Quest Publications
- 3. Instrumental methods of analysis; Willard, Merrit, Dean:7 th Edition, Chapter 25, 26
- 4. Instrumental Analysis, ; Skoog, Holler and Nieman, 5 th Edition, Chapter 31,33
- 5. Vogel's Quantitative Chemical Analysis,; 6 th Edition, Chapter 12
- 6. Analytical Chemistry Open Learning: Thermal Methods; James W. Dodd, W. James and Kenneth H. Tonge



Evaluation Scheme         Evaluation Scheme         Evaluation Scheme         Continuous Assessment (CA (Marks- 25)         NA       04       NA       02       50         NA       04       NA       02       50       5         Learning points:       .       .       Continuous Assessment (CA (Marks- 25)       Examin (Marks- 25)         Learning points:       .       .       .       Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2">Colspan="2"       Colspan="2"       .       .       .       Colspan="2"       Colspan="2"       Colspan="2"        Colspan="2" <th></th>	
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# Course Code: PRCHEMOA 504

#### **Organic Chemistry Practicals**

#### 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-phenylpyrazol-5-one
- 8. *o*-Phenylenediamine to 2-methylbenzimidazole
- 9. o-Phenylenediamine to 2,3-diphenylqunooxaline
- 10. Urea and benzil to 5,5-diphenylhydantoin

#### (Minimum 08 experiments are expected)

#### Analytical Chemistry Practicals

#### **Instrumental Experiments**

- 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.

#### **Non-Instrumental Experiments**

- 1. To carry out assay of the sodium chloride injection by Volhard's 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 number of nitro groups in the given compound usingTiCl3.

#### **References:**

Minol & Singl

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by ; A. I.

Vogels, 3rd Ed. ELBS (1964)

2. Vogel's textbook of quantitative chemical analysis, Mendham, Denny, Barnes, Thomas, Pearson education, Sixth Ed.

3. Standard methods of chemical analysis ; F. J. Welcher, 1975

4. Standard methods of chemical analysis :Instrumental methods of Analysis ; F. J. Welcher , vol. 3, 1966

5. "Standard methods of Chemical Analysis"; W. W. Scott, Vol. I, Van Nostrand

6 Spectrophotometric Determination of Traces of Metals"; E.B.Sandell and H.Onishi, ,Part 4th Ed. ,A Wiley Interscience Publication, New York,1978

# Course Codere(M 50111) Course Title:- Physical Chemistrifylective I

PROGRAM(s): M.ScI		SEMESTER	SEMESTER: I					
Course: El	ective:I	Course Code:(CHEM50111) Course Title:- Physical Chemistry-I						
Teaching S	Scheme	I			Evaluation Scheme			
Lectures (Hours Def Week)	Practical Hours Der Week)	Tutorial Hours Der Week)	Credit	Semester End (Marks-25)				
02	NA		02	50	50			
Learning C	bjectives:							
conc 2. To ap them stan	hable learners to pepts in reaction k oply the basic kno n at the workplace dards.	kinetics, molec owledge of Phy e in industry ar	ular dynar vsical chen nd academ	nics and chemical histry to perform v	rstanding of the advar thermodynamics. arious tasks assigned requirements as per esearch.			
Course Out	comes:							
	earners will app ications to ideal g	,	ed therm	odynamics, Max	well equation and it			
2. The l gase	earners will imp s, solutions, surfa	lement the ap aces and their	energetics	i.	ermodynamics to re			
	earners will und ation in the field o			ns of operators a	na schrödinger			
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4. The learners will try to accomplish a solution to problems encountered in the field of research.



## **Elective: I Physical Chemistry-I**

#### Unit - I

# Thermodynamics-I [15]

**1.1.** State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; it's 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, Schrödinger's Time independent wave equation from Schrödinger'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]



#### References: (Elective: I and II)

- 1. Peter Atkins and Julio de Paula, Atkin"s*Physical Chemistry*, 7thEdn., 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*, 3rdEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, *Physical Chemistry*, 5thEdn., Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, *Physical Chemistry*, 3rdEdn.,Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, *Text Book of Physical Chemistry*, 2ndEdn., 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, *QuantumChemistry*, 2ndEdn., 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*, 5thEdn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
- 14. Thomas Engel and Philip Reid, Physical Chemistry, 3rdEdn., Pearson Education Limited 2013.
- 15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1stEdn., 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. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
- 19. A Text book of Physical Chemistry by K L kapoor Vol 5 , 2ndEdn



#### **Elective Practical I**

PROGRAM(s): M.ScI		SEMESTER: I					
Course: Practical		Course Code: CHEM50111 Course Title:- Physical and Inorganic Chemistry Practical-I					
Teaching Sc	heme			Evaluation Scheme			
Lectures (Hours per week)	Practical (Hours per week)	Tutorial( Hours perweek)	Credit	Continuou s Assessme nt (CA)	Semester End Examination		
02	NA	-	02	25	25		

#### **Learning Objectives:**

#### **Physical Chemistry**

- 1. To Gain knowledge of the advanced concepts in pH metry. quantum mechanics, potentiometry and conductometry experiments.
- 2. To understand advance concept of thermodynamics and chemical kinetics in the chemical reactions.
- 3. To develop scientific temper and research based skills accomplish to encountered in the field of research.
- 4. To usage of subject fundamentals-principles with practical knowledge to design experiments, analyze and interpret data so as to reach to proper conclusions.
- 5. Learner will train the handling of equipments like potentiometer, conductivity meter, colorimeter and spectrophotometer.
- 6. Learner will develop scientific temper and research based skills accomplish to encountered in the field of research.

#### **Inorganic Chemistry**

- To apply basic concepts of separation and estimation of metals ions from constituent ores/alloys effectively using chemical analysis To gain knowledge of employing instrumental techniques for quantitative analysis. The learner can able to analyze structure, reactivity and reaction mechanisms of coordination 1.
- 2.
- 3.
- compounds. 4.
- It explains various methods, concepts, highlights on effect of environment on human beings. Will able to understand Commercial applications of novel materials in synthesis of 5. compounds.



# Chemistry Practical-I Course Code: CHEM 50111

#### 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 CaSO4 at room temperature.

3. To investigate the reaction between acetone and iodine.

4. 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 pKa 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, 3rdEdn., Longman Group Ltd., 1974.
- 3. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.



# Inorganic Chemistry Practical Course Code: CHEM 50111

#### **Ores and Alloys**

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

#### Instrumentation

- 1) Estimation of Fe (III) solution using Ce (IV) ions Potentiometrically
- 2) Estimation of Copper using Iodometric method Potentiometrically
- 3) Estimation of Na2CO3 in washing soda by pH metry
- 4) Estimation of Cl- ion in NaCl/KCl by Conductometry.

#### **Reference:**

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st Edn., 2010., U.N.Dhuri& 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



# Elective: II Physical Chemistry-II

PROGRAM(s): M.ScI Course: Elective-II		SEMESTER: I Course Code: (CHEM50112) Course Title:- Physical Chemistry-II					
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) 25)	Semester End Examination (Marks- 25)		
02	NA	_	02	50	50		
1. 1.To en conce 2. To appl	pts in reaction ki ly the basic know	inetics, molec	cular dynan sical chemi	nics and chemical t istry to perform var	rious tasks assigned to th		
1. 1.To en conce 2. To appl the wo	hable learners to pts in reaction ki ly the basic know prkplace in indus	inetics, molec vledge of Phys stry and acade	cular dynan sical chemi emia to me	nics and chemical t istry to perform var	thermodynamics. rious tasks assigned to the nents as per global standa		



#### Course Code:(CHEM 50112) Elective : II Physical Chemistry-II

#### Unit I

#### Chemical Kinetics and Molecular Dynamics-I [15L]

1.1. 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 **genænel** examples Organic Decompositions: Decomposition of decomposition of acetaldehyde Gas phase combustion: Reaction between hydrogen and oxygen, Semenov – Hinshelwood and Thompson mechanism, Explosion limits and factors affecting explosion limits.

- 1.2. 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.
  - 1.3.Reaction in Gas Phase

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

#### Unit II

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#### Electrochemistry [15L]

#### Recapitulation – basics of electrochemistry.

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

2.2. 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.

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

2.4. 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. Goldmann equation. (derivations are expected)

[Ref: 14 and 16, 17, 18]

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

References: (Elective: I and II)

- 1. Peter Atkins and Julio de Paula, Atkin"s*Physical Chemistry*, 7thEdn., 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*, 3rdEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, *Physical Chemistry*, 5thEdn., Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, *Physical Chemistry*, 3rdEdn.,Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, *Text Book of Physical Chemistry*, 2ndEdn., 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, *QuantumChemistry*, 2ndEdn., 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*, 5thEdn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
- 14. Thomas Engel and Philip Reid, Physical Chemistry, 3rdEdn., Pearson Education Limited 2013.
- 15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1stEdn., 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.

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- 18. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical
- Unyong Sodday Kinetics, Sara Publication, First Edition, Sept. 2022.

19 Wext book of Physical Chemistry by K L kapoor Vol 5 , 2ndEdn

#### **Elective Practical II**

PROGRAM(s): M.ScI		SEMESTER: I				
Course: Practical		Course Code: CHEM50112 Course Title:- Physical and Inorganic Chemistry Practical-I				
Teaching Sch	eme				Evaluation Scheme	
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA)	Semester End Examination	
02	NA	-	02	25	25	

#### Learning Objectives:

#### **Physical Chemistry**

- 1. To Gain knowledge of the advanced concepts
- 2. To understand advance concept of thermodynamics and chemical kinetics in the chemical reactions.
- 3. To develop scientific temper and research based skills accomplish to encounter in the field of research.
- 4. To usage of subject fundamentals-principles with practical knowledge to design experiments, analyze and interpret data so as to reach to proper conclusions.
- 5. Learner will train the handling of equipments like potentiometer, conductivity meter, colorimeter and spectrophotometer.
- 6. Learner will develop scientific temper and research based skills accomplish to encountered in the field of research.

#### **Inorganic Chemistry**

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- 1. To apply basic concepts of separation and estimation of metals ions from constituent ores/alloys effectively using chemical analysis
  - 2. To gain knowledge of employing instrumental techniques for quantitative analysis.
- 3. The learner can able to analyze structure, reactivity and reaction mechanisms of coordination compounds.

4. It explains various methods, concepts, highlights on effect of environment on human beings.

5 Will able to understand Commercial applications of novel materials in synthesis of equip of the second se

# **Elective Practical-II**

# Course Code: CHEM 50112

Physical Chemistry

#### 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 CaSO4 at room temperature.

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#### Instrumental:

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4. To verify Ostwald"s dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.

#### **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, 3rdEdn., Longman Group Ltd., 1974.
- 6. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.



# Elective Practical II Course Code: CHEM 50112 Inorganic Chemistry

#### **Ores and Alloys**

- 1) Analysis of Devarda"s alloy
- 2) Analysis of Cu Ni alloy
- 3) Analysis of Limestone.

4) Analysis of Tin Solder alloy

#### Instrumentation

- 5) Estimation of Fe (III)solution using Ce (IV) ions Potentiometrically
- 6) Estimation of Copper using Iodometric method Potentiometrically
- 7) Estimation of Na2CO3 in washing soda by pH metry
- 8) Estimation of Cl- ion in NaCl/KCl by Conductometry.

#### **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



# **Research Methodology**

	): M.Sc-I	SEMESTER: I			
Course code	e code: CHEM506 Course Title:- Research Methodolog		rch Methodology		
Teaching Sc	heme	Evaluatio			
lectures Week) Week)	ectures Veeks per Hagtical Weeks per		Tutorial Figure per Credit		Semeater End (Marks- 50)
04	-	-	04	50	50
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# **Research Methodology**

#### **Unit I Literature Survey**

#### **1.1** Print:

Primary, Secondary and Tertiary sources. Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, textbooks, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

#### **1.2** Digital:

Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, Hindex, 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.

**1.3** Information Technology and Library Resources:

The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.

#### **Unit II DATA ANALYSIS**

The Investigative Approach: Making and recording Measurements, SI units and their use, Scientific methods and design of experiments. 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

#### Unit III METHODS OF SEVENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS

Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation. 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.

#### **Unit IV CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS**

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.

#### **Reference books:-**

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), Practical skills in Chemistry, 2 nd 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 th Ed., Chapman Hill, London.

4. Harris, D. C. (2007) Quantative Chemical Analysis 6 th Ed., Freeman Chapters 3-5

analysis Cambridge University Press.

6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.

7. OSU safety manual 1.01

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PROGRAM(s): M.ScI		SEMESTER: II					
Course:Paper-I	Course:Paper-I		Course Code: <b>(CHEM508)</b> Course Title:- Inorganic Chemistry-II				
Teaching Scheme	2				Evaluation Scheme		
(Hoursper Week)	(Hours per (Hours per Week)	(Hoursper (Hoursper Week)	Credit	Continuous Assessment (Marks- 50)	Semester E (Marks- 50)		
04	NA	-	04	50	50		
Learning Object	ives:						
<b>Course Outcomes:</b> The learners will be able to study rates of reactions a the factors affecting them and understand the different techniques used study the rate of the reaction. 1. The learners will be able to learn ligand substitution reactions of Octahedral and Square planar complexes, Trans effect and factors affecting these substitution							
study the rate	will be able to	on. learn ligand si	ubstitution	reactions of Octa	niques used hedral and		
study the rate 1. The learners Square planar reactions. 2. The learners w complexes by st	will be able to complexes, Tra will be able to u udying differen	ON. learn ligand su ans effect and inderstand the it examples. Th	ubstitution d factors 18 e- and ney will als	reactions of Octa	niques used hedral and ubstitution uare planar ation and		
<ul> <li>study the rate</li> <li>1. The learners</li> <li>Square planar</li> <li>reactions.</li> <li>2. The learners was complexes by stars</li> <li>properties of a fearners was compounds like</li> </ul>	will be able to complexes, Tra will be able to u cudying differen ew selected con will understand Ziese's salt, fer	ON. learn ligand su ans effect and inderstand the it examples. Th mpounds inclu the structure a rrocene and bi	ubstitution d factors 18 e- and ney will als ding sandv and bondir s(arene)ch	reactions of Octa affecting these s 16 e- electron squ o learn the prepara vich compounds o ng of a few inorgan	niques used hedral and ubstitution lare planar ation and f Fe, Cr ic		
<ul> <li>study the rate</li> <li>1. The learners</li> <li>Square planar</li> <li>reactions.</li> <li>2. The learners with complexes by stars of a feed of a stars of a feed of a stars of a</li></ul>	will be able to complexes, Tra will be able to u cudying differen ew selected con will understand Ziese's salt, fer will understand the environme e metals have o	ON. learn ligand su ans effect and inderstand the it examples. The mpounds inclu the structure a the structure a the occurrence on the living org	ubstitution d factors 18 e- and ney will als ding sandv and bondir s(arene)ch ce and effe rent diseas ganism.	reactions of Octa affecting these s 16 e- electron squ o learn the prepara vich compounds o ng of a few inorgan romium(0) ct of toxic metals l	niques used hedral and ubstitution are planar ation and f Fe, Cr ic like Pb, As, bisoning of		

# Course Code: (CHEM 508) Course Title:-Inorganic Chemistry-II

# 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 Isomerization and racemization reactions

#### Unit II

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

**2.1.** Eighteen electron rule & electron counting with examples, sixteen electron Square Planar complexes.

2.2. Preparation and properties of the following compounds

- (a) Alkyl and aryl derivatives of Pd and Pt complexes
- (b) Carbenes and carbynes of Cr, Mo and W
- (c) Alkene derivatives of Pd and Pt
- (d) Alkyne derivatives of Pd and Pt

(e) Allyl derivatives of nickel

(f) Sandwich compounds of Fe, Cr and Half Sandwich compounds of Cr, Mo.

**2.3** Structure and bonding on the basis of VBT and MOT in the following organometallic compounds:

Zeise"s salt, bis(triphenylphosphine)diphenylacetylene platinum (0) [Pt(PPh3)2(HC $\equiv$ CPh)2], diallylnickel(diallylnickel(II), ferrocene and bis(arene)chromium(0), tricarbonyl ( $\eta$ 2-butadiene) iron(0).



Unit III Environmental Chemistry: [15 L] 3.1. Conception of Heavy Metals: Critical discussion on heavy metals 3.2. Toxicity of metallic species: a) Mercury, lead,

cadmium, arsenic, copper and chromium, with respect to their sources, distribution, speciation, biochemical effects and toxicology,

control and treatment. b) Itai-itai disease for Cadmium toxicity, c ) Arsenic Poisoning in

the Indo-Bangladesh region. **3.3. Interaction of radiation in context with the environment:** Sources and biological

implication of radioactive materials. Effect of low-level radiation on cells- Its diagnosis and treatment. Effect of radiation on cell proliferation and cancer

diagnosis and treatment, Effect of radiation on cell proliferation and cancer.

Unit IV Bioinorganic Chemistry: [15 L] 4.1. Biological oxygen carriers; hemoglobin,

hemerythrene and hemocyanine- 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 4.3. Copper containing enzymes- superoxide dismutase, 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

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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, 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. Sopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd, 2001. 10. Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd

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 McGrew Hill, New Delhi, 1993.

2. R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2nded, 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.Doughlas, 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, Caligronic, 1994.

5. G.N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, Dhuri& Sons, Calcutta, 1988.

6. J.Chem. Educ. (Special issue), Nov, 1985.

7. E.Frienden, J.Chem. Educ., 1985, 62.

8. Robert R.Crechton, Biological Inorganic Chemistry – An Introduction, Elsevier

9. J. R. Frausto da Silva and R. J. P. Williams *The Biological Chemistry of the Elements*, Clarendon Press, Oxford, 1991.

10. JM. D. Yudkin and R. E. Offord *A Guidebook to Biochemistry*, Cambridge University Press, 1980.



PROGRAM(s): M.ScI Course: Paper-II		SEMESTER: II Course Code: <b>( CHEM 509)</b> Course Title:- Organic Chemistry-II				
Teaching Sc	heme					
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)	
04	NA	-	04	50	50	
3. Accom	earning Outco	on to problem	is encount	ered in the field	of research.	
	nise the type c			e to: ediates involved	in the given orga	
-	ion and to prov	e mechanisn		eaction.		
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reacti 2) Identii subst	fy the ways to itution reaction	modify alipha ns.	n for the re atic and ar		•	
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#### Course Code: (CHEM 509) Course Title:-Organic Chemistry-II

#### 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.

#### Unit-II

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

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

**2.1.2. 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 **backinessucheophiles:** Identification of hard and soft reactive sites on the basis of MOs.

**2.1.3.** Application of FMO concepts in (a) S2 Nreaction, (b) Lewis acid base adducts (BF3-NH3 complex), (c) ethylene dimerization to Cyclobutane, (d) Diels-Alder cycloaddition, (e) regioselective reaction of allyl cation with allyl anion (f) addition of hydride to formaldehyde.

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

**2.2.1. Ultraviolet spectroscopy:** Recapitulation, UV spectra of dienes, conjugated 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).

**2.2.2. 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 III

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

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

- **3.1. Reactions:**Baylis-Hillman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction.
- **3.2. Concerted rearrangements:** Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton-Katritzky.
- **3.3. Cationic rearrangements:**Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.
- **3.4.** Anionic rearrangements: Brook, Neber, Von Richter, Wittig, Gabriel–Colman, Baker-Venkataraman.

# Unit-IV

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# <sup>1</sup>H and 13C NMR spectroscopy and Mass spectrometry (15L)

**4.1. Proton magnetic resonance spectroscopy:** Principle, Chemical shift, Factors affecting on 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,Karplusequation, long range coupling (allylic and aromatic).

**4.2. 13C 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:** Basic Principle, 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.

**G**tArcture determination involving individual or combined use of the above spectral techniques.

## **References:**

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- 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.Boydand S.K.Bhattacharjee, Pearson Publication (7thEdition)
- 5. Advanced Organic Chemistry: Reactions and mechanism, B.Millerand R.Prasad, Pearson Education.
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- 7. Understanding Organic Reaction Mechanisms, AdamsJacobs, 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, NelsonThornes.
- 10. Advanced Organic Chemistry:Reactions and mechanism, L.G.Wade,Jr.,Maya Shankar Singh, Pearson Education.
- 11. Mechanism in OrganicChemistry, eter Sykes,6th
- 12. Molecular OrbitalandOrganic chemical reactions, Ian Fleming Reference Edition, Wiley
- 13. Introduction to Spectroscopy, DonaldL.Pavia, GaryM.Lampman, GeorgeS.Kriz, Thomson Brooks.
- 14. Spectrometric Identification of Organic Compounds, R.Silverstein, G.C Basslerand T.C.Morrill, John Wiley and Sons.
- 15. Organic Spectroscopy, WilliamKemp, W.H.Freeman&Company.
- 16. Organic Spectroscopy-PrinciplesandApplications,Jagmohan,NarosaPublication.
- <sup>17.</sup> Organic Spectroscopy, V.R.Dani, TataMcGrawHillPublishingCo.
- 18. Spectroscopy of Organic Compounds, P.S.Kalsi, New Age International Ltd.
- 19. Organic Reaction Mechanisms, V.K. Ahluwalia, R.K.Parashar, Alpha Science International, 2011.
- 20. Name Reactions, Jie Jack Li, Springer
- Organic Reaction Mechanisms, V.K. Ahluwalia, R.K Parasher, Alpha Science
  International, 2011.
- Reactions, Rearrangements and Reagents by S.N. Sanyal.
- Mame Reactions, Jie Jack Li, Springer.

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- Name reactions and Reagents in Organic Synthesis, Bradford P. Mundy, M.G. Ellerd and F.G. Favaloro, John Wiley & Sons.
- 25. and F.G. Favaloro, John Wiley & Sons.
   Organic reactions and their Mechanisms, P.S. Kalsi, New Age International Publishers.
   26. Figure 10 (2014)

<sup>b.</sup> Elementary Organic Spectroscopy By- Y R Sharma, (S. Chand Publications)

	): M.ScI	SEMESTER: II					
Course: Paper-III Course Title:- A			-	CHEM 510) Analytical Chemistry-II			
Teaching Scl	heme				Evaluation Scheme		
Lectures (Hours per week)	(Hours per (Hours per (Hours Credit (CA)						
04	NA	-	04	50	50		
<ol> <li>To gain knowledge of the chromatography techniques and its applications.</li> <li>To understand application of X-ray spectroscopy for qualitative and quantitative analysis.</li> <li>To introduce radio analytical techniques.</li> <li>To apply the surface analytical techniques for system.</li> <li>To study advantages and applications of electroanalytical methods.</li> </ol>							
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# Course Code: (CHEM 510)

#### Course Title :- Analytical Chemistry-II

#### Unit I -Chromatography [15 L]

#### 1.1 Basic concepts and theories of chromatography: [5 L]

- **1.1.1** Introduction and Classification of chromatographic methods.
- **1.1.2** Concept of plate and rate theories in chromatography, efficiency, resolution, selectivity and separation capability.
- **1.1.3** Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions.

#### 1.2 Gas Chromatography: [5 L]

**1.2.1** Instrumentation –sample injection systems (split/split less), column types (solid/ liquid stationary phases), column switching techniques, temperature programming.

- **1.2.2** Requirements of an ideal detector and types of detectors in GLC and GSC.
- **1.2.3** Applications -Qualitative and quantitative analysis.

#### **1.3 High Performance Liquid Chromatography (HPLC):**[5 L]

- **1.3.1** Normal phase and reversed phase with special reference to types of commercially available columns (Use of C8 and C18 columns).
- **1.3.2** Diode array type and fluorescence detector.
- **1.3.3** Applications of HPLC.

# Unit II - Instrumental methods - II [15L]

#### 2.1 X-ray spectroscopy: [6 L]

Principle, instrumentation, applications, advantages and limitations of

- 2.1.1 X-ray absorption spectroscopy. (XAS)
- 2.1.2 X-ray fluorescence spectroscopy (XRF)
- **2.1.3** X-ray diffraction spectroscopy. (XRD)

# 2.2 Mass spectrometry: [6 L]

#### 2.2.1 Instrumentation -

i) Ion sources - electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources.

ii) Mass analyzers: Quadrupole, time of flight and ion trap.

# 2.2.2 Applications

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# 2.3 Radio analytical Methods –[3 L]

**2.3.1** Neutron Activation Analysis(NAA)- Introduction, Principle, Theory and Applications.

#### 2.3.2 Advantages and Limitations of NAA.

#### Unit III- Instrumental methods - III [15L]

# Surface Analytical Techniques – [9 L]

Principle, Instrumentation and Applications of:

- 3.1.1 Scanning Electron Microscopy (SEM)
- **3.1.2** Scanning Tunneling Microscopy (STM)
- 3.1.3 Transmission Electron Microscopy (TEM)

#### 3.2 Atomic Spectroscopy [6 L]

3.1

- **3.2.1** Atomic Spectroscopy based on plasma sources Introduction, Principle, Instrumentation and Applications.
- 3.2.2 Advantages and Limitations of AAS

## Unit IV -Electroanalytical Methods [15L]

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

(Numericals are Expected)

**4.1.1** Ion selective electrodes: Applications of - solid state, precipitate, liquid – liquid, enzyme, gas sensing, bio-catalytic membrane and enzyme-based biosensors electrodes.

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

#### 4.2 Electrogravimetry: [2 L]

- **4.2.1** Introduction, Principle and Instrumentation.
- **4.2.2** Factors affecting the nature of the deposit.
- 4.2.3 Applications.

#### 4.3 Coulometry: [3 L]

- **4.3.1** Introduction, Principle and Instrumentation.
- **4.3.2** Coulometry at controlled potential and controlled current.



#### References: Unit I

1. Instrumental Analysis, Skoog, Holler and Crouch, 7th edition

2. HPLC Practical and Industrial Applications; E.B.Sandell and H.Onishi 2 nd Ed., CRC Press

## Unit II

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- 2. Fundamentals of Radiochemistry; D. D. Sood A. V. R. Reddy and N. Ramamoorthy, , IANCAS 4th edition, 2010
- 3. Principles of Instrumental Analysis Skoog, Holler and Nieman, 5th Edition, Ch: 12, 20

# Unit III

- 1. Instrumental Analysis; Douglas A. Skoog F. James Holler Crouch, Publisher: Cengage; Edition, (2003), ISBN-10: 8131505421, ISBN-13: 978-8131505427
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  - ; Ray F. Egerton, ISBN: 978-0- 387-25800- 3 (Print) 978-0- 387-26016- 7 (Online)
- 3. Modern techniques of surface science; D.P. Woodruff and T.A. Delchar, Cambridge Univ. Press, 1994.
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- 8. Instrumental Analysis; Douglas A. Skoog F. James Holler Crouch, Publisher: Cengage; Edition (2003), ISBN10: 8131505421, ISBN-13: 978-8131505427

#### Unit IV

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- 1. Principles of Instrumental Analysis ; Skoog, Holler, Nieman, Harcourt College Publishers, 5th Edition, 1998. Chapters - 23, 24, 25.
- 2. Analytical Chemistry Principles ; John H Kennnedy, Saunders College Publishing, 2nd edition, (1990).
- 3. Modern Analytical Chemistry; David Harvey; McGraw Hill Higher education publishers, (2000).
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Rectrochemical Methods Fundamentals and Applications; Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).

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Course: Practical		Course Code: PRCHEMOA 511 Course Title:- Chemistry Practical-I (Organic Chemistry and Analytical Chemistry)				
Teaching S	cheme			Evaluation Scheme		
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)	
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## Organic Chemistry Practicals

# **Course Code: PRCHEMOA 511**

#### 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 two mixtures from each type and a total of eight mixtures are expected.)

## **Analytical Chemistry Practicals**

#### **Instrumental Experiments**

- 1. To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.
- 2. Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically.
- 3. To determine the percentage composition of HCl and H2SO4 on weight basis in a mixture of two by conductometric titration with NaOH and BaCl2.
- 4. To determine amount of potassium in the given sample of fertilizers using flame photometer by standard addition method.

#### Non-Instrumental Experiments

- 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 the break through capacity of a cation exchange resin.
- 8. Estimation of a mixture of Hydrochloric acid and boric acid by acid base titration.

#### References

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2. Vogel's textbook of quantitative chemical analysis, Mendham, Denny, Barnes, Thomas, Pearson education, Sixth Ed.

3. Standard methods of chemical analysis ; F. J. Welcher, 1975

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Company, Inc.,1939.

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# Course Codere(M 50711) Course Title:- Physical Chemistrifylective I

PROGRAM(s): M.ScI		SEMESTER: II				
Course: Elec	tive:I	Course Code: <b>(CHEM50711)</b> e:I Course Title:- Physical Chemistry-I				
Teaching Sc	heme				Evaluation Scheme	
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 25 )	Semester End Examination (Marks- 25 )	
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Learning Ol 1. To gain kn HMO theo 2. To unders: photoche 3. To develog electroche Course outc 1. To learn th box, 2D b 2. To unders	oyledge of the ory, chemical ki tand the advan mistry. o the skill to so emistry. omes ne concept of q ox, 3D box and	inetics and m iced concept lve the probl uantum cher to explain the f Schrodinge	oncepts ir nolecular s in ch ems enco mistry and	n quantum mecha dynamics. demical thermody ountered in the fig d able to solve pr	anics, application namics and eld of quantum oblems related ntum chemistry	
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# **Elective: I Physical Chemistry-I**

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

**1.1**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.

1.2. Hydrogen atom, the two particle problem, separation of the energy as translational and

potential, separation of variables, the Radial (R), Zenith (theta) and Azimuthal (Phi) equations, solution of the equation, introduction of the four quantum numbers and their interdependence on the basis of the solutions of the three equations, total wave function, expression for the energy, probability density function, distances and energies in atomic units, radial and angular plots, points of maximum probability.

1.3. 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.

1.4.Hückel Molecular Orbitals theory for ethylene, 1,3-butadiene, cyclobutadiene and benzene. (Derivation expected) [ Ref 7, 8 and 9]

#### Unit: II Photochemistry 15 L

2.1 Absorption of light, laws of photochemistry, electronic structure of molecules, molecular orbital, electronically excited singlet states, designation based on multiplicity rule, construction of Jablonski diagram, electronic transition, Frank Condon principle, selection rules, intensity of absorption bands, nature of electronic spectra and primary process, photo-dissociation, pre- dissociation.

2.2 Photo physical phenomena:

physical pathways of excited molecular system (radiative and non-radiative), phosphiorfesoerscente ordeslaged the fueresting coordentration quenching, collisional quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer between photo-excited donor and acceptor systems.

2.3. Stern-Volmer relation, critical energy transfer distances, energy transfer efficiency, examples and applications in chemical analysis. Photochemical provide the photoreduction, photored

photoisomerization and photosensitized reactions. Photochemistry of environment: Greenhouse effect.

(Ref: 17 and 18)



#### References

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- 1. Peter Atkins and Julio de Paula, Atkin"s*Physical Chemistry*, 7thEdn., 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*, 3rdEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, *Physical Chemistry*, 5thEdn., Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, *Physical Chemistry*, 3rdEdn.,Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, *Text Book of Physical Chemistry*, 2ndEdn., 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, *QuantumChemistry*, 2ndEdn., New Age International Publishers, 2000.
- 11. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press, New Delhi, 1964.
- 12. W.G. Davis, Introduction to Chemical Thermodynamics A Non Calculus Approach, Saunders, Philadelphia, 19772.
- 13. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
- 14. Ira N. Levine, *Quantum Chemistry*, 5thEdn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
- 15. Thomas Engel and Philip Reid, Physical Chemistry, 3rdEdn., Pearson Education Limited 2013.
- 16. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1stEdn., 1992.
- 17. C. H. DePuy, O. L. Chapman, Molecular reactions and photoChemistry, Prenticehall of India PVT.LTD.1988.
- 18. K. K. Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher, 1978.
- 19. Principles of physical Chemistry , Marrown and Prutton 5th edition
- 20. Essentials of Physical Chemistry ,ArunBahl, B. S Bahl, G. D.Tulli , S Chand and Co. Ltd , 2012 Edition.
- 21. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
- 22. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
- 23. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd, 2011
- 24. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan , Cambridge University Press.

#### **Elective Practical I**

PROGRAM(	s): M.ScI	SEMESTER	: I		
Course: Pra	ctical	Course Co Course Title			emistry Practical-I
TeachingSch	eme				EvaluationScheme
Lectures( Hoursper week)	Practical( Hoursper week)	Tutorial( Hoursper week)	Credit	ContinuousA ssessment(C A)	Semester EndExamination
02	NA	-	02	25	25

#### Learning Objectives:

#### **Physical Chemistry**

1. To gainknowledge of the advanced concepts in pH metry, quantum mechanics, potentiometry and conductometry experiments.

2. To develop scientific temper and research based skills accomplish to encountered in the field of research.

#### **Inorganic Chemistry**

1. The learners will be able to synthesize and characterize different inorganic coordination

complexes.

2. The learners will be trained in calculating the equilibrium constant for Fe3-/SCN1- by slope intercept method and in determining the electrolytic nature of some inorganic compounds by conductance measurements.

#### **Course Outcomes:-**

1. To use the concept of quantum chemistry to interprete the shape and information about the orbitals like 1s, 2pz and 3dz2.

2. To apply the subject fundamentals-principles with practical knowledge to design

experiments, analyze and interpret data so as to reach to proper conclusions

3. Learner will train to handle the sophisticated instrument like digital potentiometer,

conductivity meter, spectrophotometer.

#### **Inorganic Chemistry**

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The learners will characterize different coordination compounds with the help of conductivity measurements, electronic and magnetic measurements and spectroscopic measurements.

2 Able to calculating the equilibrium constant for Fe3-/SCN1- by slope intercept method 3. Able to determine the electrolytic nature of some inorganic compounds by conductance measurements.

# Elective Chemistry Practical-I Course Code: CHEM 50711

#### **Physical Chemistry**

#### Non – instrumental:

1. Polar plots of atomic orbitals such as  $\underline{1}$ s, Pz and 3*dz2* 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 Hammette constant of m- and p- amino benzoic acid/nitro benzoic acid by pH measurement.

4. To determine the Michaelis – Menten"s constant value (Km) of the enzyme Beta Amylase spectrophotometrically.

#### 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, 3rdEdn., Longman Group Ltd., 1974.

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



# Elective Chemistry Practical-I Course Code: CHEM 50711 Inorganic Chemistry

# Inorganic Preparations (Synthesis and Characterization)

- 1) Bis-(tetramethylammonium) tetrachloroCuprate (II) (Me4 N)2[CuCl4]
- 2) Bis-(tetramethylammonium) tetrachloroNickelate (II) (Me4 N)2 [NiCl4]
- 3) Bis (ethylenediammine) Copper (II) Sulphate [Cu(en)2]SO4
- 4) HexaaamineNi(II) Sulfate [Ni(NH3)6]SO4
- 5)Potassiumtrioxalato Chromate(III) K3[Cr(C2O4)3]
- 6) Tetramminemonocarbanato Cobalt (III) Nitrate [Co(NH3)4CO3]NO3

#### Instrumentation

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

#### **Reference:**

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 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



## **Elective: II Physical Chemistry-II**

PROGRAM(s	PROGRAM(s): M.ScI		2: II		
Course: Elect	tive:II	Course Code: <b>(CHEM50712)</b> Course Title:- Physical Chemistry-II			
Teaching Sc	heme				<b>Evaluation Scheme</b>
Lecture s (Hours per week)	Practica l (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 25 )	Semester End Examination (Marks-25 )
02	NA	-	02	50	50
Learning Obj	ectives:	•			

1.To gain knowledge of the advanced concepts in quantum mechanics, applications of HMO theory, chemical kinetics and molecular dynamics.

2.To understand the advanced concepts in chemical thermodynamics and photochemistry. 3.To develop the skill to solve the problems encountered in the field of quantum and electrochemistry.

# **Course outcomes:-**

1. To develop the skill to solve the problems based on molecular dynamics and quantum Chemistry.

2. Learners will able to distinguish between competitive, Noncompetitive and Uncompetitive Inhibition in enzyme-catalysed reactions.

3. Learners will get knowledge of advanced chemical kinetics and molecular dynamics.

4. Leathers will able to use advanced concepts of chemical thermodynamics in chemical reactions.



# Course Code:(CHEM50712)

Elective: II Physical Chemistry-II

#### 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  $\mathfrak{M} \mathfrak{K}^{i}$  **Real solutions:** Chemical potential in non ideal solutions excess functions of non ideal solutions calculation of partial molar volume and partial molar enthalpy, Gibbs DuhemMargules 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. [Ref 2 and 1,10,11,12]

#### Unit II

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

2.1. **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

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

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

2.4. 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, 22)



#### References

- 1. Peter Atkins and Julio de Paula, Atkin"s*Physical Chemistry*, 7thEdn., 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*, 3rdEdn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, *Physical Chemistry*, 5thEdn., Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, *Physical Chemistry*, 3rdEdn.,Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, *Text Book of Physical Chemistry*, 2ndEdn., 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, *QuantumChemistry*, 2ndEdn., New Age International Publishers, 2000.
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- 13. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
- 14. Ira N. Levine, *Quantum Chemistry*, 5thEdn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
- 15. Thomas Engel and Philip Reid, Physical Chemistry, 3rdEdn., Pearson Education Limited 2013.
- 16. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1stEdn., 1992.
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- 18. K. K. Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher, 1978.
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- 20. Essentials of Physical Chemistry ,ArunBahl, B. S Bahl, G. D.Tulli , S Chand and Co. Ltd , 2012 Edition.
- 21. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
- 22. Dr. Harichandra A Parbat and Dr. Damodar V Prabhu, Essence of Chemical Kinetics, Sara Publication, First Edition, Sept. 2022.
- 23. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd, 2011
- 24. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan , Cambridge University Press.



#### **Elective Practical II**

PROGRAM(s	): M.ScI	SEMESTER	: I		
Course: Prac	rse: Practical Course Code: CHEM50712 Course Title:- Physical and Inorg			emistry Practical-I	
TeachingSch	eme				EvaluationScheme
Lectures (Hours per week)	Practical (Hours per week)	Tutorial (Hours per week)	Credit	Continuous Assessment (CA)	Semester End Examination
02	NA	-	02	25	25

#### **Learning Objectives:**

#### **Physical Chemistry**

1. To gain knowledge of the advanced concepts in pH metry, quantum mechanics, potentiometry and conductometry experiments.

2. To develop scientific temper and research based skills accomplish to encountered in the field of research.

#### **Inorganic Chemistry**

1. The learners will be able to synthesize and characterize different inorganic coordination

complexes.

2. The learners will be trained in calculating the equilibrium constant for Fe3-/SCN1- by slope intercept method and in determining the electrolytic nature of some inorganic compounds by conductance measurements.

#### **Course Outcomes:-**

- 1. To use the concept of quantum chemistry to interprete the shape and information about the orbitals like 1s, 2pz and 3dz2.
- 2. To apply the subject fundamentals-principles with practical knowledge to design experiments, analyze and interpret data so as to reach to proper conclusions
- 3. Learner will train to handle the sophisticated instrument like digital potentiometer, conductivity meter, spectrophotometer.

#### **Inorganic Chemistry**

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**1.** The learners will characterize different coordination compounds with the help of conductivity measurements, electronic and magnetic measurements and spectroscopic measurements.

measurements. 2. Able to calculating the equilibrium constant for Fe3-/SCN1- by slope intercept method 3. Able to determine the electrolytic nature of some inorganic compounds by conductance measurements.

# Elective Chemistry Practical-I Course Code: CHEM 50712

#### **Physical Chemistry**

#### Non – instrumental:

1. Polar plots of atomic orbitals such as  $\underline{1}$ s, Pz and 3*dz2* orbitals by using angular part of hydrogen atom wave functions.

To study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate.
 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 Hammette constant of m- and p- amino benzoic acid/nitro benzoic acid by pH measurement.

4. To determine the Michaelis – Menten"s constant value (Km) of the enzyme Beta Amylase spectrophotometrically.

#### 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, 3rdEdn., Longman Group Ltd., 1974.

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



# Elective Chemistry Practical-I Course Code: CHEM 50711 Inorganic Chemistry

## Inorganic Preparations (Synthesis and Characterization)

- 1) Bis-(tetramethylammonium) tetrachloroCuprate (II) (Me4 N)2[CuCl4]
- 2) Bis-(tetramethylammonium) tetrachloroNickelate (II) (Me4 N)2 [NiCl4]
- 3) Bis (ethylenediammine) Copper (II) Sulphate [Cu(en)2]SO4
- 4) HexaaamineNi(II) Sulfate [Ni(NH3)6]SO4
- 5)Potassiumtrioxalato Chromate(III) K3[Cr(C2O4)3]
- 6) Tetramminemonocarbanato Cobalt (III) Nitrate [Co(NH3)4CO3]NO3

#### Instrumentation

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

measurement.

#### **Reference:**

- 1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 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



PROGRAM	(s): M.Sc-I	SEMESTE	R: II			
Course:Ind Training/ F	lustrial ield Projects	Course Code:CHEM512				
Teaching S	ching Scheme Evalua Schen					
Hectures Hecturs Week)	Practical Week) 08	Tutorial (Hours per week)	Credit	Continuous Assessment (CA) (Marks- 50)	Semester End Examination (Marks- 50)	
NA		-	04	50	50	
permanent To develop	students the o commitments skills in the ap	are made.	theory to	eir interest in a p practical work s ole to their caree	situations. To	befor
Course Out	comes:					
	of the Course,		_			
	Understand the Organizational Structure of a company.					
•	ork habits and ce, professiona		•	for job success ( on skills etc )	technical	
•	•	-	•	l report writing s	kills.	
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# **PROPOSED MODALITIES OF ASSESSMENT**

# **Theory Examination Pattern:**

Sr.No.	Evaluation Type	Marks
1	Written Objective/Short Answer Examination	25
2	Assignment/ Case study/ field visit report/ presentation/ project	25 t
	Total	50

#### A. Internal Assessment- 50%- 50 Marks per paper

#### B. External Examination- 50%-

#### **50 Marks per paper Semester End Theory Examination:**

- 1. Duration These examinations shall be of **two hours** duration.
- 2. Theory question paper pattern:
- a. There shall be 05 questions each of 10 marks on each unit.
- b. All questions shall be compulsory with internal choice within the questions.

#### Paper Pattern for 50 marks:

Question	Options	Marks	Questions Based on
Q.1	2 out of 4	10	Unit I Unit II
Q.2	2 out of 4	10	Unit III
Q.3	2 out of 4	10	Unit IV
Q.4	2 out of 4	10	Units
Q.5	5 out of 8	10	(I+II+III+IV)
	TOTAL	50	



#### Paper Pattern for 25 marks (Electives):

#### **25 Marks per paper Semester End Theory Examination:**

- 1. Duration These examinations shall be of **one hour** duration.
- 2. Theory question paper pattern:
- a. There shall be 02 questions each of 08 marks on each unit and one mix question for 09 marks
- b. All questions shall be compulsory with internal choice within the questions.

Question	Options	Marks	Questions Based on
Q.1	2 out of 4	08	Unit I
Q.2	2 out of 4	08	Unit II
Q.3	3 out of 6	09	Units (I+II)
	TOTAL	25	

# Semester End Practical Examination:

Particulars	Continuous assessment (CA)	Semester end external examination
Laboratory work	15	15
Viva	05	05
Journal	05	05
Total	25	25

#### **PRACTICAL BOOK/JOURNAL**

The students are required to perform 75% of the Practical for the journal to be duly certified. The students are required to present a duly certified journal for appearing at the practical examination, failing which they will not be allowed to appear for the examination.



# Letter Grades and Grade Points

Semester GPA/ Program CGPA/Semester	% Marks	Letter Grade Result
9.00-10.00	90.0-100.0	O (Outstanding)
8.00<9.00	80.0<90.0	A+ (Excellent)
7.00<8.00	70.0<80.0	A (Very Good)
6.00<7.00	60.0<70.0	B+ (Good)
5.50<6.00	55.0<60.0	B (Above Average)
5.00<5.50	50.0<55.0	C (Average)
4.00<5.00	40.0<50.0	P (Pass)
Below 4.00		F (Fail)
Ab (Absent )		Absent



# Team for Creation of Syllabus

Name	College Name	Sign
	Head, Department of Chemistry,	10
Dr. Ghanasham Bhikaji Sathe	Dapoli Urban Bank Senior Science College, Dapoli, Email:gbsathe47@gmail.com, Mobile:9420527310	Calle
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	Mahatma Phule Arts, Science and Commerce College	
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Sign of HOD

**Prof. Shivram S. Garje** Head of Department, Department of Chemistry, University of Mumbai

HEAD DEPARTMENT OF CHEMISTRY UNIVERSITY OF MUMBAI Sign of Dean,

**Prof. Shivram S. Garje** Dean, Science and Technology University of Mumbai



# Appendix B Justification for M.Sc (Organic Chemistry)

	1 2 3	The necessity for starting the course: Whether the UGC has recommended the course: Whether all the courses have commenced from the	careers in research, industry, academia, or other <b>Sherry Structure and Structure interstites</b> positive impact on the world through scientific exploration and discovery. <u>Yes</u> The course has already commenced from the academic year from 1967 and in the academic year 2022-23 it
		year 2023-24 The courses started by the University are self-financed, whether adaguate number of	is restructured under NEP 2020 This course is not self-financed. There are adequate
	4	whether adequate number of eligible permanent faculties are	PG teachers working in the colleges.
	5	available?: To give details regarding the duration of the Course and is it possible to compress the course?:	The duration of the program is two years (4 semesters). It is not possible to compress the course. Under NEP 2020 students have option of exit at the end of first year with PG Diploma in Organic Chemistry.
	6	The intake capacity of each course and no. of admissions given in the current academic year:	The intake capacity of the program is variable as per the college.
Sulla Participation of the second sec	7.	Opportunities of Employability / Employment available affer undertaking these courses:	M.Sc. (Organic Chemistry) course students have a wide range of employment opportunities across various sectors. The skills and knowledge acquired during their master's program make them well- equipped for diverse roles. Some of the common areas where M.Sc. (Organic Chemistry) course students can find employment include; Research and Development (R&D), Pharmaceutical Industry, Chemical Manufacturing, Environmental and Analytical Chemistry, Quality Assurance and Control, Materials <b>Soutence</b> and Nanotechnology, Teaching Academia, Healthcare and Clinical Research etc. The key to employability for M.Sc. (Organic Chemistry) course students is to build a strong resume through
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	inetewooskipg, hetsestrablyprojectentanid the field and Acololiticoroalsly istrayiongingpthetericdskillsh catheenhance their competitiveness in the job market.

Sign of HOD

**Prof. Shivram S. Garje** Head of Department, Department of Chemistry, University of Mumbai

HEAD DEPARTMENT OF CHEMISTRY UNIVERSITY OF MUMBAI Sign of Dean,

**Prof. Shivram S. Garje** Dean, Science and Technology University of Mumbai

