YEAR-WISE AND SEMESTER-WISE DISTRIBUTION OF SUBJECTS
DEPARTMENT OF ORGANIC CHEMISTRY–M.Sc.
FIRST SEMESTER
ACADEMIC YEAR 2019-20 OF 2018-20 BATCH (CBCS)

Sl. No.	Part	Subject Code	Title of the Subject	Hours /Week	Duration of Exam (hrs)	Marks			Credits
						Internal	External	Total	
1	I	MOC16101	*Communicative competence (AECC-1)	2	2	20	30	50	2
2	II	MOC16102	Inorganic Chemistry-I (CORE-1)	4	3	40	60	100	4
3	II	MOC16103	Organic Chemistry-I (CORE-2)	4	3	40	60	100	4
4	II	MOC16104	Physical Chemistry-I (CORE-3)	4	3	40	60	100	4
5	II	MOC16105	Analytical Techniques And Spectroscopy -I (CORE-4)	4	3	40	60	100	4
	PRACTICALS								
6	II	MOC16151	Inorganic Chemistry Practical-I (CORE-1)	6	4	30	45	75	3
7	II	MOC16152	Organic Chemistry Practical-I (CORE-2)	6	4	30	45	75	3
8	II	MOC16153	Physical Chemistry practical-I (CORE-3)	6	4	30	45	75	3
	Total			**36**	**-**	270	405	675	**25**

*Ability Enhancement Compulsory Course (AECC) (Not included in CGPA)

YEAR-WISE AND SEMESTER-WISE DISTRIBUTION OF SUBJECTS

DEPARTMENT OF ORGANIC CHEMISTRY– M.Sc.

SECOND SEMESTER

ACADEMIC YEAR 2019-20 OF 2018-20 BATCH (CBCS)

Sl. No.	Part	Subject Code	Title of the Subject	Hours /Week	Duration of Exam (hrs)	Marks			Credits
						Internal	External	Total	
1	I	MOC16201	*Value Education and Personality Development (AECC-2)	2	2	20	30	50	2
2	II	MOC16202	Inorganic Chemistry-II (CORE-5)	4	3	40	60	100	4
3	II	MOC16203	Organic Chemistry-II (CORE-6)	4	3	40	60	100	4
4	II	MOC16204	Physical Chemistry-II (CORE-7)	4	3	40	60	100	4
5	II	MOC16205	Analytical Techniques And Spectroscopy -II (CORE-8)	4	3	40	60	100	4
	PRACTICALS								
6	II	MOC16251	Inorganic Chemistry Practical-II (CORE-5)	6	4	30	45	75	3
7	II	MOC16252	Organic Chemistry Practical-II (CORE-6)	6	4	30	45	75	3
8	II	MOC16253	Physical Chemistry practical-II (CORE-7)	6	4	30	45	75	3
	Total			**36**	**-**	270	405	675	**25**

*Ability Enhancement Compulsory Course (AECC) (Not included in CGPA)

YEAR-WISE AND SEMESTER-WISE DISTRIBUTION OF SUBJECTS

DEPARTMENT OF ORGANIC CHEMISTRY–M.Sc.

THIRD SEMESTER

ACADEMIC YEAR 2019-20 OF 2018-20 BATCH (CBCS)

Sl. No.	Part	Subject Code	Title of the Subject	Hours /Week	Duration of Exam (hrs)	Marks			Credits
						Internal	External	Total	
1	I	MOC19301	*Computer Applications (AECC-3)	2	2	20	30	50	2
2	II	MOC19302	Organic Chemistry-III (CORE-9)	4	3	40	60	100	4
3	II	MOC19303	Organic Chemistry-IV (CORE-10)	4	3	40	60	100	4
4	II	MOC19304	Organic Chemistry-V (CORE-11)	4	3	40	60	100	4
5	II	MOC19305A MOC19305B	Heterocyclic Chemistry / Green Chemistry (DSE-1)	4	3	40	60	100	4
	PRACTICALS								
6	I	MOC19351	*Synthesis and Estimation of Drugs (SEC-1)	5	4	30	45	75	3
7	I	MOC19352	*Seminar (SEC-2)	2	1	-	25	25	1
8	II	MOC19353	Organic Chemistry Practical-III (CORE-9)	5	4	30	45	75	3
9	II	MOC19354	Organic Chemistry Practical-IV (CORE-10)	6	4	30	45	75	3
Total				**36**	**-**	270	430	700	**26**

*Ability Enhancement Compulsory Course (AECC) (Not included in CGPA)
* Skill Enhancement Course (SEC)
* Discipline-Specific Elective (DSE)

YEAR-WISE AND SEMESTER-WISE DISTRIBUTION OF SUBJECTS

DEPARTMENT OF ORGANIC CHEMISTRY–M.Sc.

FOURTH SEMESTER

ACADEMIC YEAR 2019-20 OF 2018-20 BATCH (CBCS)

Sl. No.	Part	Subject Code	Title of the Subject	Hours /Week	Duration of Exam (hrs)	Marks			Credits
						Internal	External	Total	
1	II	MOC19401	Organic Chemistry-VI (CORE-12)	4	3	40	60	100	4
2	II	MOC19402A MOC19402B	*Natural Products /Bioorganic Chemistry (DSE-2)	4	3	40	60	100	4
3	II	MOC17402A MOC17402B	*Analytical Methods/ Nano & Polymer Chemistry (GE)	4	3	40	60	100	4
	PRACTICALS								
3	I	MOC17451	*Seminar (SEC-3)	2	1	-	25	25	1
4	II	MOC17452	Project	22	1	80	120	200	9
5	III	-	*PLANET (Outreach)	-	-	-	-	-	1
Total				36	-	200	325	525	22

*Skill Enhancement Course (SEC)
* Discipline-Specific Elective (DSE)
*Generic Elective (GE)
* Programme of Loyola Academy for Neighborhood Empowerment & Transformation (PLANET) (Not included in CGPA)

COMPUTER APPLICATIONS

Credits: 2 **Semester: III**

Subject code: MOC19301 **No. of lecture hours: 30**

Objective: To study the applications of computer and its techniques in Organic Chemistry.

UNIT-I **6 Hrs**

Basics in Computers-I

- History of computers, generations of computers 1
- Characteristics of computers 1
- Data representation – number system 1
- Binary, octal and hexadecimal 1
- Conversion from one number system to another 1
- Hardware, Software, Translators, Compilers and interpreters 1

UNIT-II **6 Hrs**

Basics in Computers-II

- System software, application software 1
- Simple operating concepts, flowchart 1
- Algorithms with simple examples 1
- DOS commands – Internal and external commands 2
- File management and directory structure 1

UNIT-III **6 Hrs**

Windows and MS-Word

- Working with windows explorer 1
- Creating a new directory, copy files from one directory to another, deleting files. 1
- Control panel- background, Mouse settings, screen saver 1
- Creating a new document, designing documents setting margins, headers and footers, tabs & tables 1
- Formatting a document editing – find and replace text 1
- Protecting documents, Mail Merge and Newsprint. 1

Unit–IV **6 Hrs**

Power Point and Excel

- Creating, opening and saving presentations 1
- Working on different views -Working with slides 1
- Formatting paragraphs, drawing and working with objectives 1
- Creating a new worksheet-select, edit (Copy, move, format, setting column width etc.) 1
- Referencing cells (Addressing methods). 1
- Functions-logical, mathematical, statistical, date and time, formulae, charts, macros. 1
- Creating an excel database-sort and filter database. Performing what –if analysis on worksheet data. 1
- Analysis data with pivot tables 1

Unit-V **6 Hrs**

Access

- Access basics: Database, tables, records, fields 1
- The database window: Tables, Queries, forms, reports, Macros, and modules 1
- Creating a table, setting field properties, modifying the structure, setting primary key, adding and deleting fields 1
- Entering table data. Creating forms 1
- Queries on data- select query, update query, delete Query, Append query 1
- Designing reports 1

Suggested Reading:

1. Deepak B. 2012. **Fundamentals of Information Technology**. New Delhi: Excel Books Publishers

2. Sharon C. and Neil J. S. **ABCs of Windows**. New Delhi: BPB Publications.

ORGANIC CHEMISTRY-III

Credits: 4 **Semester: III**

Subject Code: MOC19302 **No. of lecture hours: 60**

Objectives:

- To understand the conformational analysis of cyclic system.
- To enable the student to apply the knowledge of stereochemistry in asymmetric synthesis.
- To impart knowledge to students regarding various synthetic routes for synthesis of compounds.
- To impart knowledge to student regarding the new techniques developed in organic synthesis

UNIT-I **12 Hrs**

Conformational Analysis (Cyclic systems):

- Study of conformations of cyclohexane, mono, di *substituted* cyclohexane. 4
- Cyclohexene, cyclohexanone (2-alkyl and 3-alkyl ketone effect), and 2-halo cyclohexanones. 2
- Stereochemistry of decalins, bicyclo-(3,3,0)-octane and hydrindanes. 1
- Conformational structures of piperidine, *N*-methylpiperidine, D-Glucose (Pyranose and Furanose). 1
- Conformational effects on the stability and reactivity of diastereomers in cyclic molecules - steric and stereoelectronic factors – examples. 2
- Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. 1
- Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring. 1

UNIT-II **12 Hrs**

Asymmetric Synthesis-I:

- Introduction and terminology: Topocity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces-symmetry, substitution and addition criteria. 2
- Prochirality nomenclature: Pro-R, Pro-S, Re and Si. 1
- Selectivity in synthesis: Stereospecific reactions (substrate stereoselectivity). 3

Stereoselective reactions (product stereoselectivity): Enantioselectivity and diastereoselectivity. Conditions for stereoselectivity: Symmetry and transition state criteria.

- % Enantiomer excess, % enantioselectivity, optical purity, % diastereomeric excess and % diastereoselectivity. 1
- Techniques for determination of enantioselectivity: Specific rotation, chiral ^{1}H NMR and chiral HPLC. 2
- Classification of asymmetric reactions substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1,2-asymmetric induction, Cram's rule and Felkin-Anh model. 3

UNIT-III **12 Hrs**

Asymmetric Synthesis-II:

- Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, evans oxaenolates, azaenolates. Chiral sulfoxides. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder. 4
- Asymmetric aldol reaction, Diastereoselective Aldol reaction and its explanation by Zimmerman Traxel model. Auxiliary controlled Aldol reaction. Double diastereoselection-matched and mismatched aldol reactions. 2
- Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2 BH and $IPCBH_2$. Reductions with CBS reagent. 2
- Chiral catalyst controlled asymmetric synthesis: Sharpless, Jacobsen and Shi asymmetric epoxidations. Sharpless asymmetric dihydroxylation and amino hydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysts. Chiral catalyst controlled Diels-Alder reactions. 4

UNIT-IV **12 Hrs**

Synthetic strategies:

- Terminology: target, synthon, synthetic equivalent, functional group interconversion, retrosynthetic analysis. 2

- Crieteria for selection of target. 1
- Linear and convergent synthesis. 1
- Synthesis involving chemoselectivity, regioselectivity, reversal of polarity 2
  Strategic bond: Criteria for disconnection of strategic bonds.
- Importance of the order of events in organic synthesis: Salbutamol, Proparacaine. 1
- One group and two group C-X disconnections. 1
- One group C-C disconnections. Alcohol and carbonyl compounds. 1
- Two group C-C disconnections: Diels-Alder reaction, 1,2 and 1,3-difunctionalised compounds. 2
- Synthesis of (+) Disparlure by retro synthetic approach. 1

UNIT-V **12 Hrs**

New Techniques and concepts in organic synthesis:

- Solid phase polypeptide synthesis and requirements 2
- Solid phase oligonucleotide synthesis (Phospharamidite method). 1
- Strategies in oligosaccharide synthesis (Linear and convergent synthesis). 1
- Kahne glycosidation. 1
- Tandem synthesis-Electrocyclic Diels- Alder reaction. 1
- Baldwin rules 2
- Phase transfer catalyst: Crown ethers and quaternary ammonium salts. 2
- Combinatorial synthesis-introduction, definition and types: Haughton's tea bag procedure, Furkas mix and split Method. 2

Suggested Reading:

1. Eliel, E.L. and Wilen, S.H. 2008. **Stereochemistry of Carbon Compounds.** John Wiley & Sons INC.
2. Nasipuri, D. 2006. **Stereochemistry of Organic Compounds, Principles & Applications**. 2nd Edition. New Delhi: New Age International Publishers.
3. Kalsi, P.S. 2010. **Stereochemistry: Conformation & Mechanism.** 7th Edition. New Delhi: New Age International Publishers.
4. Ward, R.S. 1999. **Stereoselectivity in Organic Synthesis**. John Wiley & Sons INC.
5. Nogardy, M. 1987. **Asymmetric Synthesis.** VCH. Publishers.

6. Carruthers, W. 2004. **Some Modern Methods of Organic Synthesis.** 4th Edition. Cambridge University Press.
7. Jagadamba, Singh and Yadav, L.D.S. 2011. **Organic Synthesis.** New Delhi: Pragathi Prakasan Publications.
8. Meckie, R. K., Smith, D. M. and Atken, R. A. 1990. **Guidebook to Organic Synthesis**. 2nd Edition.
9. Warren, S. 2002. **Organic Synthesis-The Disconnection Approach**. John Wiley& Sons.
10. Michael B Smith. 1994. **Organic Synthesis**. MacGraw Hill International Editions.

ORGANIC CHEMISTRY-IV

Credits: 4 **Semester: III**

Subject Code: MOC19303 **No. of lecture hours: 60**

Objectives:

- To acquire knowledge about the organometallic reagents.
- To emphasise the importance of regioselectivity through protection of various functional groups
- To impart knowledge of new synthetic routes developed for organic synthesis
- To gain knowledge about advanced techniques in NMR

UNIT-I **12 Hrs**

Protecting groups

- Protection of alcohols by ethers, silyl ether and ester formation. 2
- Protection of 1,2-diols by acetals, ketals and carbonate formation. 2
- Protection of amines by acetylation, benzoylation, benzyloxycarbonyl, butyloxy carbonyl, fmoc and triphenyl methyl groups. 3
- Protection of carbonyl compounds by acetal, ketal and thioacetal formation. 2
- Protection of carboxylic acids by ester and ortho ester (OBO) formation. 3

UNIT-II **12 Hrs**

Organometallic reagents and Applications

- Organo magnesium reagents (Grignard reagents). 2
- Organo lithium reagents. 2
- Organo copper reagents. 2
- Organo borane reagents. 2
- Organo phosphorus reagents: Wittig reagent, modified Wittig reagent 2
- Mannich reaction and Robinson annulation. 1
- Stork-enamine reaction and Shapiro reaction. 1

UNIT-III **12 Hrs**

New synthetic reactions

- Baylis-Hillman reaction. 1
- Julia-Lythgoe olefination. 1

- Peterson's stereoselective olefination. 1
- Mukayama aldol reaction. 1
- Mitsunobu reaction, McMurrey reaction 1
- Heck reaction 1
- Buchwald-Hartwig coupling, Suziki coupling 1
- Stille coupling, Sonogishira coupling 1
- Eishenmosher-Tanabe fragmentation 1
- Aza-Cope and Aza-Wittig reaction 1
- Ugi reaction 1
- Click reaction 1

UNIT-IV **12 Hrs**

^{13}C NMR

- CW and PFT techniques. 1
- Types of ^{13}C NMR spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. 4
- ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. 2
- Homonuclear (^{13}C,^{13}C-J) and Heteronuclear (^{13}C,^{1}H-J and ^{13}C,^{2}H-J) coupling. 3
- Applications of ^{13}C NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. 1
- ^{13}C NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods. 1

UNIT-V **12 Hrs**

2D NMR and ORD

- Principles of 2D NMR 1
- Classification of 2D-experiments. 1
- 2D-J-resolved spectroscopy. 1
- Homonuclear and Heteronuclear 2D-J-resolved spectroscopy. 1

- Correlation spectroscopy (COSY) Homo COSY (^{1}H-^{1}H COSY) Hetero COSY (^{1}H,^{13}C COSY, HMQC): 2-Pentanone and Ethyl benzoate 2
- NOESY: Sodium 2-methyl acrylate 1

ORD:

- Plain curves and anomalous curves, optical rotation, circular birefringence, circular dichroism and cotton effect. 2
- Octant rule, axial halo ketone rule, Application of octant rule to study the absolute configuration and conformations of 3-methyl cyclohexanone, Menthone, Cis-10-methyl-2-decalone. 3

Suggested Reading:

1. Michael B Smith. 1994. **Organic Synthesis**. MacGraw Hill International Editions.
2. Jagadamba Singh and Yadav, L.D.S. 2011. **Organic Synthesis.** Pragathi Prakasan Publications.
3. Meckie, R.K., Smith, D. M. and Atken, R. A. 1990. **Guidebook to Organic Synthesis**. 2nd Edition.
4. Carruthers, W. 2004. **Some Modern Methods of Organic Synthesis**. 4th Edition. Cambridge University Press.
5. Willis, C and Willis, M. 1995. **Organic Synthesis.** Oxford University press
6. Jie Jack Li. 2006. **Name Reactions**. 3rd Edition. Springer International Edition.
7. Francis, A. Carey. 2008. **Organic Chemistry**. 7th Edition. McGraw Hill International Editions.
8. Silverstein, R.M., Bassler, G.C. and Morrill, T.B. 2006. **Spectroscopic Identification of Organic Compounds.** 6th Edition. John Wiley & Sons.
9. William Kemp. 2008. **Organic Spectroscopy.** 3rd Edition. Palgrave.
10. Kalsi, P S. 2005. **Spectroscopy of Organic Compounds**. 6th Edition. New Delhi: New Age International publishers.
11. Pavia, 2004. **Introduction to Organic Spectroscopy**. 3rd Edition. Thomson.
12. Jagmohan. 2010. **Organic Spectroscopy, Principles and Applications**. 2nd Edition. New Delhi: Narosa Publication House Pvt. Ltd.

Organic Chemistry V

Credits: 4 **Semester: III**
Subject Code: MOC19304 **No. of lecture hours: 60**
Objectives:

- To emphasize the existence and importance of natural products and heterocyclic compounds beneficial to mankind.
- To students learn about green methods of synthesis and new synthetic reactions
- To acquire knowledge about nanomaterial and their importance

UNIT-I **12 Hrs**

Natural Products

- Isolation of natural products by steam distillation, solvent extraction and chemical methods. 2
- Definitions, medical importance, occurrence**,** detections by various color tests, Classification of alkaloids and terpenoids 2
- Isoprene rule, Special isoprene rule. 1
- General methods in structural determination of terpenes. 1
- Structure determination and synthesis of α-terpeniol and camphor. Structure determination and synthesis of β- carotene. 4
- General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine. 2

UNIT-II **12 Hrs**

Heterocyclic chemistry

- Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms. 2
- Synthesis and reactivity of indole, benzofuran and benzothiophene. 4
- Synthesis and reactivity of quinoline, isoquinoline, coumarin, chromone. 6

UNIT-III **12 Hrs**

Formation of –C=C-, –C=N-, –C=O-, and –C≡N-, bonds:

- **C=C:** Tebbe Reagent, Bamford-Stevens Reaction and Nickel (II) Catalyzed Cross-Coupling with Grignard Reagents (Kumada Reaction).
- Introduction to extrusion reactions, extrusion of N_2, CO, CO_2, SO_2
- **C=N:** Addition of Grignard reagent to nitriles, ylides to nitorso compounds, pyrolysis of alkyl and aryl azides, rearrangement of trityl N-haloamines and hydroxyl amines (Stieglitz rearrangement)
- **C=O:** Pyrolysis of β-hydroxy alkenes,
- **C≡N:** Dehydration of unsubstituted amides, oximes and its derivatives

UNIT-IV **12 Hrs**

Nano chemistry

- Introduction, definition of a nanosystem, dimensionality and size dependent phenomena, Surface to volume ratio, Fraction of surface atoms, Surface energy and surface stress- surface defects **2**
- Preparation of nanoparticles – Bottom-up approach, To-down approach, chemical vapour deposition method, Thermolysis method, Pulsed laser method **2**
- Carbon-based nano materials (buckyballs, nanotubes, graphene), Metal based nano materials (nanogold, nanosilver and metal oxides). Core-shell **4**

nanoparticles, self- assembled monolayers, magnetic nanoparticles.

- Characterisation of Nanomaterials: UV-Visible spectroscopy, SEM, TEM, STM, XRD (principles only). **3**
- Applications of nanomaterials in medicine. 1

UNIT-V **12 Hrs**

Introduction to Green Chemistry

- Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis. 4
- Green alternatives of organic synthesis: coenzyme catalyzed reactions 2
- Green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalyzed synthesis. 4
- Condensation reactions, Green photochemical reactions 2

SUGGESTED READING:

1. Finar, I.L. 2009. **Textbook of Organic Chemistry**. Vol II. 5th Edition. Pearson Publications.
2. Bhat, S.V. and Nagasampangi, B.A. 2009. **Chemistry of Natural Products**. New Delhi: New Delhi: Narosa Publishing House.
3. Kalsi, P.S. 1983. **Chemistry of Natural Products.** Kalyani Publishers.
4. Gilchrist, T. 1987. **Heterocyclic Chemistry.** Pitmann Publishing Ltd.
5. Bansal, R. K. 2005. **Heterocyclic Chemistry**. 4th Edition. New Delhi: New Age International Pvt. Ltd.
6. Joule J.A. and Mills, K. 2004. **Heterocyclic Chemistry**. 4th Edition. Blackwell Publishers.
7. Joule J.A. and Smith. 2010. **Heterocyclic Chemistry**. 5th Edition. ELBS.
8. Acheson. R. M. 1967. **An Introduction to the Chemistry of Heterocyclic Compounds.** 2nd Edition. Wiley & Sons.
9. Gupta R R. Kumar, M. and Gupta V. 2005. Vol-I and Vol-II.**Heterocyclic Chemistry**. 1st Indian Edition Springer publications.
10. Michael B Smith. 1994. **Organic Synthesis**. MacGraw Hill International Editions.
11. Jagadamba Singh and Yadav, L.D.S. 2011. **Organic Synthesis.** Pragathi Prakasan Publications.
12. Meckie, R.K., Smith, D. M. and Atken, R. A. 1990. **Guidebook to Organic Synthesis**. 2nd Edition.

13. Carruthers, W. 2004. **Some Modern Methods of Organic Synthesis**. 4th Edition. Cambridge University Press.
14. Willis, C and Willis, M. 1995. **Organic Synthesis.** Oxford University press
15. Pradeep, T. 2007. **Nano: the Essentials**. Tata McGraw Hill.
16. Varghes, T. and Balakrishna, K. M. 2012. **Nanotechnology**. Atlantic publishers.
17. V. K. Ahluwalia, M. Kidwai. 2004. **New Trends in Green Chemistry**. Anamaya Publishers.
18. Ahuluwalia, V.K. 2006. **Green Chemistry, Environmental Benign Reactions.** New Delhi: Ane Book Publications.
19. Sanghi R. and Srivastava, M.M. 2003. **Green Chemistry, Environment Friendly Alternatives**. New Delhi, Narosa Publications.

HETEROCYCLIC CHEMISTRY

Credits: 4 **Semester: III**

Subject Code: MOC19305A **No. of lecture hours: 60**

Objectives:

- To enable the student to understand and appreciate the importance of heterocyclic compounds
- To understand the mechanism involved in the synthesis and applications of heterocyclic compounds.

UNIT-I **12 Hrs**

Fused heterocyclics

- Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms. 4
- Synthesis and reactivity of indole, benzofuran 4
- Synthesis and reactivity of benzothiophene, quinoline, isoquinoline, coumarin, chromone. 4

UNIT-II **12 Hrs**

Non aromatic heterocyclics

- Different types of strains, interactions and conformational aspects of nonaromatic heterocyclics 3

- Synthesis, reactivity, and importance of the following ring systems of Azirines, Aziridines,Oxiranes, Thiiranes — 5
- Synthesis, reactivity, and importance of the following ring systems of Azetidines, Oxetanes, Thietanes — 4

UNIT-III **12 Hrs**

Five and six membered heterocyclic with two hetero atoms

- Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Isoxazole, Isothiazole. — 3
- Imidazole, Oxazole, Thiazole. — 3
- Benzimidazole, Benzoxazole and Benzthiazole. — 3
- Pyridazine, Pyrimidine. Pyrazine. — 2
- Oxazine, thiazine — 1

UNIT-IV **12 Hrs**

Heterocyclics with more than two hetero atoms

- Synthesis, reactivity, aromatic character and importance of the following Heterocycles:
- 1,2,3- triazoles, 1,2,4-triazoles. Tetrazoles. — 3
- 1,2,4-oxadiazole, 1,3,4-oxadiazole 1,2,5- oxadiazole. — 3
- 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles. — 3
- 1,2,3-triazine, 1,2,4- triazine, 1,3,5- triazine, tetrazines. — 2
- Synthesis and importance of Purines and Pteridines. — 1

UNIT-V **12 Hrs**

Large ring and other Heterocyclics

- Synthesis, structure, stability and reactivity of following Heterocyclics
- Azepines, Oxepines and Thiepines. — 3
- Diazepines rearrangements of 1,2 - diazepines. — 1
- Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonines. — 4
- Selenophenes, Tellerophenes, Phospholes and Boroles. — 4

Suggested Reading:

1. Gilchrist, T. 1987. **Heterocyclic Chemistry.** Pitmann Publishing Ltd.
2. Bansal, R. K. 2005. **Heterocyclic Chemistry**. 4th Edition. New Delhi: New Age International Pvt. Ltd.
3. Joule J.A. and Mills, K. 2004. **Heterocyclic Chemistry**. 4th Edition. Blackwell Publishers.
4. Joule J.A. and Smith. 2010. **Heterocyclic Chemistry**. 5th Edition. ELBS.
5. Acheson. R. M. 1967. **An Introduction to the Chemistry of Heterocyclic Compounds.** 2nd Edition. Wiley & Sons.

GREEN CHEMISTRY

Credits: 4 **Semester: III**

Subject Code: MOC19305B **No. of lecture hours: 60**

Objectives:

- To introduce the concept of Green Chemistry
- To impart knowledge about different methods of Green Synthesis
- To acquire knowledge about ionic–liquids and polymer supported synthesis and multicomponent reactions

UNIT-I **12 Hrs**

Introduction to Green Chemistry

- Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis. 3
- Green alternatives of organic synthesis: coenzyme catalyzed reactions 2
- Green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalyzed synthesis. 5
- Condensation reactions, Green photochemical reactions 2

UNIT-II **12 Hrs**

Use of Ultrasound and Microwaves in Organic Synthesis

- Use of ultrasound**:** Introduction, instrumentation, the phenomenon of cavitation. 2
- Sonochemical esterification, substitution, addition, alkylation, oxidation, reduction and coupling reactions. 2
- Use of Microwaves: Introduction, concept, reaction vessel/medium, specific effects, atom efficiency (% atom utilization), advantages and limitations. 2
- *N*-alkylation and alkylation of active methylene compounds, condensation of active methylene compounds with aldehydes and amines. 2
- Diels-Alder reaction. Deprotection of esters and silyl ethers. Oxidation of alcohols and sulfides. 2
- Green chemistry in the pharmaceutical industry: Ibuprofen manufacture, biocatalysis. 2

UNIT-III **12 Hrs**

Ionic-liquids and Polymer supported reagents in organic synthesis

- Introduction, structure, synthesis and applications of some important ionic liquids in organic synthesis. 3
- Introduction- properties of polymer support, advantages of polymer supported reagents and choice of polymers. 2
- Applications: Substrate covalently bound to the support: Dieckmann cyclisation. 2
- Preparation of polymer bound aldehyde and application in aldol and Wittig reactions. 2
- Synthesis of polystyryl boronic acid and use in diol protection reaction. 1
- Reagent linked to a polymeric material: Preparation of sulfonazide polymer and application in diazotransfer reaction. 2
- Synthesis of polymer bound per acid and its applications. 1
- Polymer supported catalytic reactions: Preparation of polymer supported $AlCl_3$ and application in etherification and acetal formation reactions. 2

UNIT-IV **12 Hrs**

Phase transfer catalysis and crown ethers

- Phase transfer catalysis: Introduction, definition, mechanism of phase transfer catalysis. Types of phase transfer catalysts and reactions and their advantages. 3
- Preparation of catalysts and their application in substitution, elimination, addition, alkylation, oxidation and reduction reactions. 3
- Crown ethers: Introduction, nomenclature, features, nature of donor site. General synthesis of crown ethers. 2
- Synthetic applications: Alkylation, generation of carbenes, aromatic substitution and displacement reactions. 2
- Generation and application of superoxide anions. Cation deactivation reactions. 2

UNIT-V **12 Hrs**

Multi-component Reactions

- Studies on the mechanistic aspects and use of the following reactions in organic synthesis: 4
- Passerini-Ugi; Hantsch; Biginelli; Doebner-Miller
- Ritter; Jacobson; Betti; Robinson-Schopf; 3
- Barbier; Baylis-Hilmann; Ivanov and Suzuki coupling reaction. 5

Suggested Reading:

1. Ahuluwalia, V.K. 2006. **Green Chemistry, Environmental Benign Reactions.** New Delhi: Ane Book Publications.
2. Sanghi R. and Srivastava, M.M. 2003. **Green Chemistry, Environment Friendly alternatives**. New Delhi: Narosa Publications.
3. Dehmlov, E.V. and Dehmlov, S.S. 1983. **Phase Transfer Catalysis.** 2nd Edition. Verlagchemie, Wienheim.
4. Mathur, N.K. Narang C. K. and Williams, R. E. 1980. **Polymers as Aids in Organic Synthesis.** New York: Academic Press.

SEMINAR

Credits: 1 **Semester: III**

Subject Code: MOC19351 **No. of lecture hours: 2 hr/week**

Objectives:

- To make the student to understand and present the topics in the subject related to Chemistry in a class room.
- The components in the mode of presentation include

1) Economy of time

2) Voice as a tool of communication

3) Blackboard use and teaching aids

4) Language and diction

5) Relating to the audience

SYNTHESIS AND ESTIMATION OF DRUGS

Credits: 3 **Semester: III**

Subject Code: MOC19352 **No. of lab hours: 5 hrs/ week**

Objectives:

- To enable the student to develop analytical skill in organic quantitative analysis
- To understand the techniques involved in the preparation of standard solutions, standardization and calculations in the estimations of compounds.

Isolation of the following natural products:

- Piperine from pepper (Soxhlet extraction)
- Eucalyptus oil from leaves (steam distillation)

Synthesis of the following drugs:

- Phenacetin
- Phenytoin
- Benzocaine
- Chlorbutol
- 4-Aminobenzene sulfonamide.

- FIuorescein
- Antipyrine
- Proponolol

Estimation of the following drugs:

- Assay of Ibuprofen
- Assay of Ascorbic acid
- Chloride in Ringer's lactate (argentometry)
- Riboflavin (colorimetry)

Suggested Reading:

1. Mann and Saunders. 2009. **Practical Organic Chemistry.** Pearson education.
2. Vogel. 2000. **A Textbook of Practical Organic Chemistry**. Vol 1 and 2
3. Ahuluwalia, V. K. 2006. **Green Chemistry, Environmental Benign Reactions**. New Delhi: Ane Book Publications.

ORGANIC CHEMISTRY III- PRACTICAL

Credits: 3 **Semester: III**

Course Code: MOC19353 **No. of lab hours: 5 hrs/ week**

Objectives:

- To enable the student to develop analytical skill in organic qualitative analysis and to develop preparative skills in organic preparations involving two or three stages.
- To enable to students to understand the mechanism involved in the name reactions and conditions of the reactions involving the preparations.

Synthesis of

- Vanillyl alcohol from vanillin ($NaBH_4$ reduction)
- 7-Hydroxy coumarin (Pechman synthesis)
- 4- Chlorotoluene from 4-toluidine (Sandmeyer reaction)
- Benzilic acid from benzoin (Benzilic acid rearrangement)
- Benzpinacol (photoreduction) and Benzpinacol to Benzpinacolone (Rearrangement)
- *Trans*-azobenzene to *cis*-azobenzene (Photoisomerisation: Monitored by Uv-visible spectroscopy)

- Preparation of allylic alcohols *via* Baylis-Hillman reaction using DABCO as a catalyst

or

- 7-Hydroxy-3-methyl flavone (Baker –Venkatraman reaction)
- 2,4,6-Trimethyl quinolone (Skraup synthesis)
- Cinnamic acid (Condensation)
- Dihydropyrimidines (MCR, Biginelli reaction)
- Caprolactam (Beckmann rearrangement)

Suggested Reading:

1. Mann and Saunders. 2009. **Practical Organic Chemistry.** Pearson education.
2. Vogel's **A Textbook of Practical Organic Chemistry**. Vol 1 and 2
3. Ahuluwalia, V. K. 2006. **Green Chemistry, Environmental Benign Reactions**, New Delhi: Ane Book Publications.
4. Kappe, C. O. 1997. **Dihydropyrimidine Synthesis (Beginilli reaction)**. *J. Org. Chem*. 62 (21), 7201–7204.

ORGANIC CHEMISTRY IV- PRACTICAL

Credits: 3 **Semester: III**

Subject Code: MOC19354 **No. of lab hours: 6hrs/week**

Objectives: To learn and apply the principles of spectroscopy for the study and structural elucidation of molecules.

- Identification of 25 unknown organic compounds by interpretation of IR, UV, ^{1}H NMR, ^{13}C NMR and mass spectra.
- **Chemistry software programmes:** Chem Draw (10 structures), analysis of IR and NMR using ACD/1D NMR processor. EXCEL: Drawing graphs.

Suggested Reading:

1. Silverstein., Bassler and Morrerl, 1998. **Spectrometric Identification of Organic Compounds.** 5th Edition. John Wiley& sons.
2. Field, L.D., Sternhell, S. and Kalman J. R. **Organic Structures from Spectra**. 5th Edition. John Wiley & sons.

ORGANIC CHEMISTRY V

Credits: 4 **Semester: IV**

Subjected Code: MOC19401 **No. of lecture hours: 60**

Objectives: To impart knowledge to the students regarding drug design and its mechanism of action

UNIT-I **12 Hrs**

Principles of Drug design and drug discovery

- Introduction to drug discovery, pharmacognosy, pharmacokinetics (ADME) pharmacodynamics. 4
- Lead discovery- from natural products, folklore drugs, natural hormones and neurotransmitters, emitting drugs (me too drugs) 2
- Serendipitous discovery of leads e.g.Penicillin and Librium. 1
- Definition and principles of design of agonists (Eg: Salbutamol,) and antagonist (Eg: Cimitidin) 3
- Principles of prodrug design. 2

UNIT-II **12 Hrs**

SAR and QSAR studies

- Binding role of hydroxy group, amino group, aromatic ring, double bond, ketones and amides. 1
- Lead modification strategies: Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion or contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead and rigidification of lead. conformational blockers 3
- Structure pruning techniques in lead modification e.g. morphine. 1
- Discovery and design of oxaminquine, and captopril. 2
- Structure-Activity Relationship studies in benzodiazepines. 1
- Introduction to Quantitative- Structure Activity Relationship studies. QSAR parameters- pKa, logp, Lipophilicity substituent constant, Hammett substitutent constant, Taft's constant and their relationship with biological activity. 2
- Multiparameter QSAR- Hansch analysis, Craig's plot, Topliss method. 2

UNIT-III **12 Hrs**

Drugs acting on metabolic processes, cell walls and specific enzymes.

- Different types of classification of drugs. 1
- Introduction to macromolecular targets. 1
- Introduction to enzymes and enzyme inhibitors 1
- Folate metabolism in bacteria, Antifolates: Structural formulae of sulfaguanidine, dapsone and trimethoprim. Synthesis and mechanism of action of Sulfamethoxazole. 2
- Structural formulae β-Lactams antibiotics: penicillin-G, cephalosporin-C, Cefalexin and amoxacillin. 2
- Synthesis and mechanism of action of penicillin-G, cephalosporin-C . 1
- Inhibitors of ACE, H^+/K^+ ATPase enzymes: Synthesis and mechanism of action of Captopril, Enalapril, Omeprazole. 4

UNIT-IV **12 Hrs**

Drugs acting on Ionchannels and receptors

- Introduction to ion channels; Cell membrane 1
- Drugs acting on Ca^{+2}, Na^{+} and K^{+} channels and their mode of action. 1
- Structural formulae of Diltiazem, Tetracaine and 4-aminopyridine Synthesis of Diltiazem. 1
- Introduction to nervous system and structure of neurons. 1
- Definition and examples of agonists, antagonists, neurotransmitters, receptors. 1
- α- Adrenergic receptor agonists and antagonists. Structural formulae of Epinephrine, Nor-epinephrine, Methyldopa and Terazosin. Synthesis of norepinephrine. 1
- β- Adrenergic receptor agonists and antagonists. Synthesis of Salbutamol, propronolol. 1
- Cholinergic-receptor agonists and antagonists-structural formula of acetyl choline, Succinyl choline, Atropine. Synthesis of succinyl choline. 2
- Dopamine receptor agonists and antagonists Synthesis of L-Dopa and Chlorpromazine. 2
- Serotonin receptor agonists and antagonists-Structural formulae of Serotonin and Metaclopramide. 1
- Histamine receptor agonists and antagonists-Structural formulae of Histamine, Chloropheneramine, Ranitidine and Cimetidine. 1

UNIT-V **12 Hrs**

Drugs acting on genetic material and Immune system

- Introduction to nucleic acid; structure functions
- DNA-intercalating agents: Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Chloroquine. 1 2
- DNA-Binding and Nicking agents: Synthesis of Metronidazole, Tinidazole and Dimetridazole. 2
- DNA-Polymerase inhibitors: Synthesis of AZT 1
- Inhibitors of transcribing enzymes: Structural formulae of Rifamycins and

partial synthesis of Rifampicin. 2

- Drugs interfering with translations: Structural formulae of Erythromycin, Chloromycetin, Tetracyclines and Amino glycosides. Synthesis of Chloromycetin. 2
- Immunosupressing agent-structural formula and mechanism of action of Cyclosporin. Immunoenhancers-use of vaccines. 2

Suggested Reading:

1. Manfred E. Wolf. 1995. **Burger's Medicinal Chemistry and Drug Discovery.** 5th Edition. John Wiley & Sons.
2. Graham L. Patrick. 2001. **Introduction to Medicinal Chemistry.** 2nd Edition. Oxford University Press.
3. R.B.Silverman. 1992. **Organic Chemistry of Drug Design & Drug Action.** 2nd Edition. Academic Press.
4. Thomas Nogardy. 1988. **Biochemical Approach to Medicinal Chemistry.** 2nd Edition. Oxford University Press.
5. Kadam 2005. **Principles of Medicinal Chemistry.** 13th Edition. Vol. I &II, Nirali Prakashan Publishers.
6. Gareth Thomas. 2004. **Medicinal Chemistry: An Introduction.** John Wiley & Sons
7. Daniel Ledneiser. 2009. **Strategies for Organic Drug Synthesis and Design**. 2nd Edition. John Wiley & Sons Publishers.
8. Rama Rao N. 2001. **Principles of Organic Medicinal Chemistry**. New Delhi: New Age International Publishers.
9. William Foye. 2013. **Principles of Medicinal Chemistry.** 7th Edition. Lippincott Williams and Wilkins Publishers.
10. Ashutoshkar. 2005. **Medicinal Chemistry.** 3rd Edition. New Delhi: New Age International Publishers.

ADVANCED NATURAL PRODUCTS

Credits: 4 **Semester: IV**

Subject Code: MOC19402A **No. of lecture hours: 60**

Objectives:

- To emphasize the existence and importance of natural products beneficial to mankind.
- To students learn about biosynthetic methods of natural products
- To acquire knowledge about structural elucidation of natural products

UNIT-I **12 Hrs**

Natural Products-II / ALKALOIDS AND TERPENOIDS

- Isolation, structural elucidation, stereochemistry and synthesis of
- **Quinine** 2
- Morphine 5
- Abeitic acid 3
- β-Amyrin 2

UNIT-II **12 Hrs**

Natural Products-III/ STEROIDS AND HORMONES

- Occurrence, isolation, structure determination, stereochemistry and total synthesis of Cholesterol 6
- Structure determination and synthesis of
- Androsterone 2
- Progesterone 2
- Stereochemical structure and biological activity of Testosterone, Estrone, Estradiol and Aldosterone 2

UNIT-III **12 Hrs**

Natural Products-IV/ PROSTAGLANDINS

- Occurrence, classification and physiological activity of prostaglandins 2
- Structure determination and synthesis of
- PGE1α 2
- PGE2α 2
- PGE3α 2
- Structure determination and synthesis of rotenone 4

UNIT-IV **12 Hrs**

Natural Products-V/ PLANT PIGMENTS

- Classification of pigments 1
- Occurrence, Isolation, structural elucidation and synthesis of 3
- Apigenin (Flavone)
- **Luteolin/Myricetin (Flavone)** 2
- **Diadzein (Flavonols)** 2
- Classification, isolation and properties of Anthocyanins 1
- Structural elucidation and synthesis of Cyanidin-7-arabinoside 3

UNIT-V

Biosynthesis of Natural Products

- Introduction to biosynthesis and biogenesis. 1
- Difference between Laboratory synthesis and biosynthesis. 1
- Methods for determination of biosynthetic mechanism. Feeding experiments – use of radioisotopes Measurement of incorporation– absolute incorporation, specific incorporation. Identification of position of labels in labeled natural products by chemical degradation and spectral methods. 2
- Major biosynthetic pathways:
- Mevalonic acid pathway: Biosynthesis of α-terpeniol and camphor 2
- Acetate-Malonate pathway: Biosynthesis of aromatic compounds: Eugenone, pholroglucinol, orsinol and rubrofusarin. 3
- Shikimic acid pathway: Biosynthesis of essential amino acids–phenylalanine, tyrosine, tryptophan and morphine. 3

SUGGESTED READING:

1. Finar, I.L. 2009. **Textbook of Organic Chemistry**. Vol II. 5th Edition. Pearson Publications.
2. Bhat, S.V. and Nagasampangi, B.A. 2009. **Chemistry of Natural Products**. New Delhi: New Delhi: Narosa Publishing House.
3. Kalsi, P.S. 1983. **Chemistry of Natural Products.** Kalyani Publishers.
4. Rashmi Jain, Alok Sahai, Sandhya Pimplapure, Usha Soni, 2016. **Chemistry of Natural Products**. Pragati Prakashan

BIO ORGANIC CHEMISTRY

Credits: 4 **Semester: IV**

Subject Code: MOC19402B **No. of lecture hours: 60**

Objectives:

- To introduce to biomolecules of importance carbohydrate, proteins, nucleic acids, lipids and enzymes
- To emphasize on the structure reactivity of enzymes and their mechanisms

UNIT-I **12 Hrs**

Carbohydrates and Proteins

- Carbohydrates: Determination of relative and absolute configuration in D (+) Glucose. 1
- Occurrence, importance and synthesis of monosaccharides containing functional groups such as amino, halo and sulphur. 2
- Structural elucidation and synthesis of sucrose. Conformational structures of D (+) ribose, 2-deoxy-D-ribose, sucrose, lactose, maltose and cellobiose. 4
- Structural features of starch and cellulose. 2
- Proteins: Acid and enzymatic hydrolysis of proteins. 1
- Determination of the amino acid sequence in polypeptides by end group analysis. Chemical synthesis of di and tri peptides. Merrifield's solid phase synthesis. 2

UNIT-II **12 Hrs**

Nucleic acids and Lipids

Introduction: Structural formulae of bases, nucleosides, nucleotides, and base pairing. 2

- Synthesis of nucleoside and nucleotides 2
- Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA. 2
- Replication, transcription and translation. Synthesis of nucleosides and nucleotides. 2
- Structure and synthesis of acylglycerols, phosphoglycerides and

sphingolipids. 4

UNIT-III **12 Hrs**

Enzymes and their action

- Definition. Classification based on mode of action. 1
- Enantiomer discrimination by Three- point Contact model. Factors affecting enzyme catalysis. Enzyme inhibition- reversible and irreversible inhibition. Immobilized enzymes. 2
- Transition state theory and Acid-Base catalysis. 1
- Covalent catalysis- Binding modes of catalysis (i) Proximity effect (ii) Transition state stabilization (iii) Strain and Distortion. 4
- Examples of some typical enzyme mechanisms for (i) Triose phosphate isomerase, (ii) α-chymotrypsin and serine protease (iii) Lysozyme (iv) Carboxy peptidase-A (v) Ribonuclease. 4

UNIT-IV **12 Hrs**

Enzyme Models and Enzymatic transformations

- Introduction: Biomimetic chemical approach to biological systems- Enzyme models Advantage of enzyme models, requirements necessary for the design of enzyme models. 3
- Host-guest complexation chemistry. Examples of some host molecules- crown ether cryptanes, cyclodextrins. cyclodextrin based enzyme models-calixarenes, ionophores, micelles and synzymes (synthetic enzymes)-chiral recognition and catalysis. 5
- Introduction to industrial enzymes. 1
- Enzymatic synthesis of α-amino acids and peptides. 1
- Transformations of lipases and esterases. 2

UNIT-V **12 Hrs**

Coenzymes

- Introduction. cofactors, cosubstrates, prosthetic groups.classification: Vitamin derived coenzymes and metabolite coenzymes. 2
- Structure and biological functions and mechanism of reactions catalysed coenzyme A 1

- Thiamine pyrophosphate, pyridoxal phosphate (PLP) 1
- Nicotinamide adenosine dinucleotide/their phosphates 1
- Flavin adenine nucleotide FAD, $FADH_2$ and Flavin mononucleotide (FMN, $FMNH_2$) 2
- Lipoic acid, biotin, 1
- Tetrahydrofolate, Ubiquinone. 1
- Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), 1
- S-adenosyl methionine (SAM) 1
- Uridine di phospho sugars (UDP-sugars) 1

Suggested Reading:

1. Fersht and Freeman. 1985. **Enzyme Structure and Mechanism.** 2nd Edition. New York: Springer Publication.
2. Hennan Dugas. 1999. **Bio-Organic Chemistry: A Chemical Approach to Enzyme Action.** New York: Springer Publication.
3. D L Nelson and Cox, M.M. 2013. **Lehninger Principles of Biochemistry.** Freeman publications.
4. Conn and Stumpf. 2006. **Outlines of Biochemistry**. 5th Edition. John Wiley & Sons INC.

ANALYTICAL METHODS

Credits: 4 **Semester: IV**

Subject Code: MOC19403A **No. of lecture hours: 60**

Objectives:

- To provide a sound knowledge in chromatographic techniques in the separation and identification of components from biological sources.
- To understand the basic principle of analytical chemistry in the preparation of solutions, standardization ion and preservation ion.
- To understand the techniques involved in the instrumental analysis particularly in electro analytical, UV-visible, fluorescence and ^{1}H NMR spectral methods

UNIT-I	**12 Hrs**
GC and HPLC	12
• Gas Chromatography: Principles, Gas-Solid (GC, Adsorption) and Gas – Liquid (GLC, partition) chromatography.	2
• Performing GC separations & Instrumentation – Stationary phases, carrier gases	2
• Detectors (FID), Temperature selection, Applications of GC.	2
• High Perfomance Liquid Chromatograpahy (HPLC): Principles, stationary phases, solvents and columns for HPLC	3
• Instrumentation, normal phase (NPC) and reverse-phase chromatography (RPC), Detector (UV, refractive index) and applications HPLC	3
UNIT-II	**12 Hrs**
GC-MS, LC-MS	
• GC-MS: Principle, instrumentation	2
• Interfaces, jet separators, Mass analyzer (Quadrupole), Mass chromatogram with an example, applications	4
• LC-MS: Principles, Instrumentation	3
• Interfaces (APCI, ESI) and applications.	3

UNIT-III **12 Hrs**

Electro analytical Methods

- Types and Classification of Electro analytical Methods. 2
- Potentiometry: Types of electrodes, Hydrogen gas, Calomel, Quinhydrone and glass electrodes. Determination of pH. Potentiometric titration of redox reaction. 5
- Conductometry: Definition of terms: Conductivity, specific conductivity, cell constant, mobility of ions. Conductometric titration of weak acid against strong base. 5

UNIT-IV **12 Hrs**

UV-Vis and Fluorescence Spectroscopy

- Preparation of solutions: Percentage by weight, volume and strength. Normality, molarity, ppm and ppb 2
- Classification of electronic transitions, Terminology: Chromophore, Auxochrome, Types of shifts, Isosbestic point 1
- Lambert and Beers Law, verification, deviations, and Molar absorption coefficients, Substituent and solvent effects 4
- Principle, origin of fluorescence and phosphorescence spectra, types of relaxation processes, variables affecting fluorescence and phosphorescence spectra, excitation spectra and emission spectra. 5

UNIT-V **12 Hrs**

^{1}H NMR Spectroscopy

- Principles of NMR. Instrumentation: pulsed FT instrumentation 3
- Equivalent and non-equivalent protons, enantiotopic and diastereotopic protons, signal integration. 2
- Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects. 4
- Spin-spin coupling: vicinal, and germinal, coupling constants. 1
- ^{1}H NMR of ethanol, ethyl acetate, 3-pentanone, toluene and aniline. 2

Suggested Reading:

1. Sane and Joshi. 1 999. **Electro analytical Chemistry Theory and Applications.** Quest Publications.
2. Raymond PW Scott. **Techniques and Practices of Chromatography.** New York: Marcel Dekker, Inc.
3. Banwell and Mc Cash. 1966. **Fundamentals of Molecular Spectroscopy.** McGraw-Hill.
4. Silverstein, R.M., Bassler, G.C. and Morrill, T.B. 2006. **Spectroscopic Identification of Organic Compounds.** 6th Edition. John Wiley & Sons.
5. William Kemp. 2008. **Organic Spectroscopy.** 3rd Edition. Palgrave.
6. Kalsi, P S. 2005. **Spectroscopy of Organic Compounds**. 6th Edition. New Delhi: New Age International publishers.
7. Pavia. 2004. **Introduction to Organic Spectroscopy**. 3rd Edition. Thomson.
8. Jagmohan. 2010. **Organic Spectroscopy, Principles and Applications**. 2nd Edition. New Delhi: Narosa Publication House Pvt. Ltd.

NANO AND POLYMER CHEMISTRY

Credits: 4 **Semester: IV**

Subject Code: MOC19403B **No. of lecture hours: 60**

Objectives:

- To introduce the students to the concept of Nanochemistry, different types of nanomaterials and their applications in various fields
- To introduce students to concept of green chemistry
- To acquire the knowledge about different types of environmental pollution

UNIT-I **12 Hrs**

Nanochemistry I

• Introduction, Scientific revolutions, Time and length scale in structures, Definition of a nanosystem, Dimensionality and size dependent phenomena, Surface to volume ratio, Fraction of surface atoms, Surface energy and surface stress- surface defects, Properties at nanoscale (optical, mechanical, electronic and magnetic).	6
• Classification based on dimensionality-Quantum Dots, Wells and Wires	
• Carbon-based nano materials (buckyballs, nanotubes, graphene), Metalbased nano materials (nanogold, nanosilver and metal oxides). Core-shell nanoparticles, self- assembled monolayers, magnetic nanoparticles.	6

UNIT-II **12 Hrs**

Nanochemistry II

• Characterisation by powder XRD method Qualitative applications of	1
• nanomaterials in Solar energy conversion and catalysis	1
• Nanoelectronics, applications in displays and other devices, Nanomaterials for data storage, chemical and biosensors	4
• Nanomaterials in food and agriculture	1
• Nanomaterials in communication, environmental protection	2
• Nanomedicine and Nanobiotechnology	3

UNIT-III **12 Hrs**

Polymer Chemistry

- Introduction to polymers, basic concepts: monomers, repeat units, degree of polymerization. Linear, branched and network polymers. 3
- Classification of polymers. Polymerization: condensation, addition, radical chain-ionic and co-polymerization. 3
- Molecular weight determination and control of molecular weight 1
- Polymerization in homogeneous and heterogeneous systems. 2
- Ziegler-Natta polymerization with mechanism, Stereo regulated polymers, syndiotactic, isotactic and atactic polymers. 3

UNIT-IV **12 Hrs**

Green Chemistry

- Basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis. 3
- Green alternatives of organic synthesis: coenzyme catalyzed reactions. 2
- Use of Microwaves: Introduction, concept, reaction vessel/medium, use of ultrasound: Introduction, example electrophilic aromatic substitution reactions, oxidation-reduction reactions, condensation reactions. 5
- Ionic liquids: Introduction and applications in organic synthesis, examples 2

UNIT-V **12 Hrs**

Environmental Chemistry

- Introduction to environmental pollutions. 1
- Chemistry of Atmosphere: Composition and structure of atmosphere, Greenhouse effect, Ozone depletion, Photochemical smog, Air sampling techniques, Sources, effects and monitoring of air pollutants by Instrumental methods, Control of air pollution. 5
- Water Pollution, Different types of water pollutants, Sources, characteristics and effects of water pollutants, Monitoring of Water Pollutants (mercury and lead), Treatment of Municipal Waste Water, and 6

Treatment of Industrial Waste Water.

Suggested Reading:

1. Pradeep, T. 2007. **Nano: the Essentials**. Tata McGraw Hill.
2. Varghes, T. and Balakrishna, K. M. 2012. **Nanotechnology**. Atlantic publishers.
3. V. K. Ahluwalia, M. Kidwai. 2004. **New Trends in Green Chemistry**. Anamaya Publishers.
4. Ahuluwalia, V.K. 2006. **Green Chemistry, Environmental Benign Reactions.** New Delhi: Ane Book Publications.
5. Sanghi R. and Srivastava, M.M. 2003. **Green Chemistry, Environment Friendly Alternatives**. New Delhi, Narosa Publications.
6. Dehmlov, E.V. and Dehmlov, S.S. 1983. **Phase Transfer Catalysis.** 2nd Edition. Verlagchemie, Wienheim.
7. Mathur, N.K., Narang C. K. and Williams, R. E. 1980. **Polymers as Aids in Organic Synthesis.** New York: Academic Press,
8. Ballini, R. 2009. **Eco-Friendly Synthesis of Fine Chemicals.** RSC Publications.
9. Sodhi. G.S. 2005. **Fundamental Concepts of Environmental Chemistry.** 2nd Edition. New Delhi: Narosa publishing House.
10. Rao M. N. and Datta, A. K. 2007. **Waste Water Treatment.** 2nd Edition. Oxford Publications.

SEMINAR

Credits: 1 **Semester: IV**

Subject Code: MOC19451 **No. of lecture hours: 2 hr/week**

Objectives:

- To make the student to understand and present the topics related to recent research topic to chemistry.
- The components in the mode of presentation include

1) Economy of time

2) Voice as a tool of communication

3) Blackboard use and teaching aids

4) Language and diction

5) Relating to the audience

PROJECT

Credits: 9 **Semester: IV**

Subject Code: MOC19452 **Duration: 65 working days/ 3 Months**

Objectives:

- To enable the student to develop analytical skill in organic reactions, qualitative analysis and to develop preparative skills in multi-step organic synthesis.
- To enable to students to understand the mechanism involved in the multi-step organic synthesis and conditions of the reactions involving the preparations.

Subject offered for GE

M.Sc. Organic Chemistry:

1. Analytical Methods

2. Nano and Polymer Chemistry

M.Sc. Biotechnology:

1. Application of Biotechnology

2. Biostatistics

M.Sc. Food Technology:

1. Food and Nutrition

2. Food Processing and Quality Control

COMMUNICATIVE COMPETENCE

Credits: 2 **I Year/ I Semester**

Subject code: MOC16101 **No. of lecture hours: 30**

Objectives:

- English language course will help students to develop a natural and accurate style of English pronunciation.
- English language course will also improve your ability to express ideas clearly and confidently in English.

Outcome

- Student is able to apply the knowledge of communicative competence to express the ideas clearly.

Unit -01:	**6hrs**
• Features of Indian English	1
• Correction of sentences, Structures	1
• Tenses, ambiguity - idiomatic distortions	1
• Informal conversation Vs Formal expression	1
• Verbal and non-verbal communication	1
• Barriers to effective communication – kinesics	1
Unit -02: Types of Communication	**6hrs**
• Oral, aural, Writing and reading	1
• Word-Power - Vocabulary- Jargon –	1
• Rate of speech, pitch, tone- Clarity of voice	1
• Technical presentations	1
• Types of presentation ,video conferencing	1
• Participation in meetings - chairing sessions	1
Unit -03:	**6hrs**
• Formal and informal interviews	1
• Ambiance and polemics	1
• Interviewing in different settings and for different purposes	1
• e.g., eliciting and giving information	1
• Recruiting, performance appraisal	1
• Group discussions, curriculum vitae	1
Unit -04:	**6hrs**
• Written communication	2
• Differences between spoken and written communication	2
• Features of effective writing such "as clarity, brevity	1
• Appropriate tone clarity, balance etc.	1
Unit -05:	**6hrs**
• Letter-writing business letters –	1
• pro forma culture - format - style – effectiveness, promptness	1
• Analysis of sample letters collected from industry –email, fax.	1
• Technical Report writing –Business and Technical Reports	1
• Types of reports - progress reports, routine reports, annual reports - format –	1
• Analysis of sample reports from industry –Synopsis and thesis writing	1

References:

1. Rajendra Pal, J S KorlahaHi, **Essentials of Business Communication**, Sultan Chand & Sons, New Delhi.
2. Andrea J. Rutherford, **Basic Communication Skills for Technology**, Pearson Education Asia, Patparganj, New Delhi-92.
3. V. Prasad, **Advanced Communication Skills**, Atma Ram Publications, New Delhi.
4. Raymond V. Lesikav; John D. Pettit Jr.; **Business Communication; Theory & Application**, All India Traveller Bookseller, New Delhi-51.
5. R. K. Madhukar, **Business Communication**, Vikas Publishing House Pvt. Ltd.

INORGANIC CHEMISTRY-I

Credits: 4 **I Year/I Semester**

Subject Code: MOC16102 **No. of lecture hours: 60**

Objectives

- To impart knowledge of co-ordinate complexes, their reaction mechanisms and their stabilities.
- To acquire the knowledge of symmetry and assigning the same to the molecules.

Outcome

- The student will have the knowledge of symmetry of coordinate complexes, stabilities and their reaction mechanism.

Unit 01: Bonding in metal complexes-I **12 hrs**

- Crystal Field Theory: Salient features of CFT. Splitting pattern of d-orbital in regular Octahedral, tetrahedral, trigonal planar and linear geometries. **6**
- John-Tellar Theorem- tetragonally distorted octahedral, square planar **1**
- Factors influencing the magnitude of crystal field splitting in octahedral complexes – nature of metal ions, nature of ligands, geometry. **4**
- Concept of weak field and strong field - Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate complexes. **1**

Unit 02: Symmetry of molecules-I **12 hrs**

- Concept of Symmetry in Chemistry–Symmetry Operations **2**
- Symmetry Elements: Rotational Axis of Symmetry and Types of Rotational Axes, Plane of Symmetry and types of Planes, Improper Rotational Axis of Symmetry, Inversion Center and Identity Element. **4**
- More about Symmetry Elements-Molecular Point Groups: Definition and Notation of Point Groups **1**
- Classification Molecules in to C_1, C_s, C_i, C_n, C_{nv}, C_{nh}, $C_{\alpha v}$, D_n, D_{nh}, D_{nd}, $D_{\alpha h}$, S_n (n=even) **5**

Unit 03: Reaction mechanism-I **12 hrs**

- Labile and Inert Complexes. VBT Explanation of Lability and Inertness. Taube's Explanation of Lability and Inertness **2**
- Ligand substitution reactions: Energy profile of a reaction – Transition state or Activated Complex. **1**
- Types of substitution reactions: SE: Electrophilic substitution reaction, S_N1: Substitution, Nucleophilic, Unimolecular Mechanism (Dissociative Mechanism), S_N2: Substitution, Nucleophilic, Bimolecular Mechanism (Associative Mechanism), S_N1CB: Substitution, Nucleophilic, Unimolecular Conjugate Base Mechanism. **4**
- Ligand substitution reactions in octahedral complexes: Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis, Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of S_N1CB Mechanism. **4**
- Substitution reactions without Breaking Metal-Ligand bond. **1**

12 hrs

Unit 04: Coordination equilibria

- Solvation of metal ions- Binary complexes: Formation of binary metal complexes and their stability **1**
- Types of Stability Constants– relation between them- trends in Step-wise Stability Constants (Factors causing decrease and increase in Step-wise Stability) **1**
- Factors influencing the stability constants: (i) Ligand effects: Basicity, Substituent, Steric, Chelate (size and number of chelate rings), Macro cyclic and Cryptate effects; (ii) Metal ion effects: Ionic potential, Effective Nuclear charge and Atomic Number (Irving-William's Order), geometry of metal ion and ligand–chelate effect and its thermodynamic origin. **5**
- Jahn-Tellar effect on Stability constants of metal complexes **1**
- Pearson's Theory of Hard and Soft Acids and Bases (HSAB), Applications of HSAB, Electro negativity *vs* Hardness and Softness. Symbiosis. **2**
- Methods used for the determination of stability constants (Basic Principles only): Spectrophotometric method. **2**

Unit 05: Ligational aspects of diatomic molecules **12hrs**

- Metal Carbonyls: Carbon monoxide as a ligand, molecular orbital of CO, donor and acceptor molecular orbital of CO; bonding modes of CO: terminal and bridging. **4**
- Evidence for multiple bonding from bond lengths and stretching frequencies, 18 valence electron rule and its application. **2**
- Metal Nitrosyls: NO as a ligand, molecular orbital of NO, donor and acceptor components; bonding modes of NO: terminal (linear, bent) and bridging; structural aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$. **4**
- Stereochemical control of valance in $[Co(diars)_2(NO)]^{+2}$ and $[Co(diars)_2(NO)(SCN)]^{+1}$. **2**

References:

Unit-01:

1. J. E. Huheey, K. A. Keiter and R. L. Keiter, 1993, **Inorganic Chemistry** (4th Ed), Harper Cotton's College Publications.
2. G. L. Eichorn, *Inorganic Biochemistry*, **1982**, Vol 1, Elsevier.

Unit-02:

3. Mark Ladd**,** 2000, **Symmetry and Group theory in Chemistry**, Marwood Publishers, London, Mark Ladd.
4. K.Veera Reddy, 1999, **Symmetry and Spectroscopy of Molecules** (1st Ed.), New Age International (P) Limited.

Unit-03:

5. Mark Ladd, 2000, **Symmetry and Group theory in Chemistry,** Marwood Publishers, London.
6. K. Veera Reddy, 1999, **Symmetry and Spectroscopy of Molecules** (1st Ed), New Age International (P) Limited.
7. F. Albert Cotton, 2009, **Chemical Applications of Group Theory** (3rd Ed), Wiley India.

Unit-04& 05:

8. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 1999, **Advanced Inorganic Chemistry** (6th Edn), Wiley Interscience.
9. M. M. Taqui Khan and A. E Martell, 1974, **Homogeneous Catalysis by Metal complexes** Vol I, Academic Press NewYork.

10. D. F. Shriver, H. D. Kaerz and R. D. Adams, 1990, **The Chemistry of Metal Cluster Complexes.** Oxford University Press, NewYork.

ORGANIC CHEMISTRY-I

Credits: 4 **I Year/I Semester**

Subject Code: MOC16103 **No. of lecture hours: 60**

Objectives

- To impart the knowledge of stereochemistry.
- To understand the mechanisms in organic reactions.
- To apply the knowledge of reactive intermediates and apply the same for various molecular rearrangements.
- To understand the conformational analysis of acyclic system.

Outcome

- The student will be able to have understanding of the reaction mechanisms, rearrangements, Stereochemistry and conformations of organic molecules.

Unit- 01: Stereochemistry **12 hrs**

- Molecular representation of Fischer, Newman, Sawhorse, Wedge projections and their interconversion. **1**
- Molecular symmetry and chirality: Symmetry operations and symmetry elements (C_n & S_n). Criteria for chirality and desymmetrisation **1**
- Axial, planar and helical chirality, configurational nomenclature: Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, and atropoisomerism. Planar chiral ansa compounds and trans- cyclooctene. Helically chiral compounds. **3**
- Relative and absolute configuration: Determination of absolute configuration. Anomalous X-ray scattering method and chemical correlation methods. **3**
- Racemization, racemates and resolution techniques: Resolutions by direct crystallization, diastereoisomer salt formation, chiral chromatography and asymmetric transformation. **2**
- Determination of configuration in *E, Z*-isomers: Spectral, chemical methods of configuration determination of *E, Z*-isomers. **2**

Unit- 02: Reaction mechanism-I **12 hrs**

- Effect of structure on reactivity: brief review of inductive effect, electromeric effect, resonance effect, hyper conjugation, steric effect. **2**
- Electrophilic addition to carbon carbon double bond: Stereo selective addition to carbon carbon double bond; antiaddition: bromination and epoxidation followed by ring opening. Syn addition of OsO_4 and $KMnO_4$, Prevost and Woodward oxidation. **3**
- Elimination reactions: E_2, E_1, E_1CB mechanisms. Orientation and stereoselectivity in E_2 eliminations. Pyrolytic syn elimination and α-elimination, elimination *Vs* substitution **4**
- Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping and crossover experiments. **3**

Unit- 03: Reactive intermediates **12hrs**

Generation, detection, structure, stability and reactions of **4**

- Carbocations (Classical and Non-Classical) carbanions
- Carbenes, nitrenes **4**

- Free radicals **2**
- Benzyne **2**

Unit- 04: Molecular rearrangements **12hrs**

- Molecular rearrangements: Definition and classification. Molecular rearrangements involving electron deficient carbon: Wagner- Meerwein, Pinacol-Pinacolone, Allylic and Wolf rearrangement. **3**
- Electron deficient nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements **4**
- Electron deficient oxygen: Baeyer-Villiger oxidation. **2**
- Base catalysed rearrangements: Benzilic acid, Favourski, Transannular, Sommlett-Hauser and Smiles rearrangement, Von-Richter rearrangements **3**

Unit- 05: Conformational Analysis (Acyclic Systems) **12 hrs**

- Introduction to conformational isomerism and concept of dynamic stereochemistry. Klyne-Prelog terminology for conformers and torsion angles. **1**
- Conformational analysis of ethane, 1,2-disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane-2,3-diol, amino alcohols and 1,1,2,2-tetrahalobutanes. Conformations of unsaturated acyclic compounds: propylene, 1-Butene, acetaldehyde, propionaldehyde and butanone. **6**
- Conformational diastereoisomers and conformational enantiomers. Factors affecting the conformational stability and conformational equilibrium: Attractive and repulsive interactions. Use of physical and spectral methods in conformational analysis. **3**
- Conformational effects on the stability and reactivity of acyclic diastereoisomers, steric and stereo electronic factors with examples. **2**

References:

Unit-01 & 05:

1. Ernest L Eliel, Samuel H.Wilen, 2008, **Stereochemistry of Carbon compounds**, John Wiley & Sons INC.
2. D. Nasipuri, 2006, **Stereochemistry of organic compounds- Principles and Applications** (2nd Ed.), New Age International publishers.
3. P S Kalsi, 2010, **Stereochemistry: Conformation & Mechanism** (7th Ed.), New Age International publishers

Unit-02, 03& 04:

4. Petersykes, **A guidebook of mechanism of organic chemistry** (6th Ed.), Pearson Education, India.
5. Jerry March, 1992, **Advanced Organic Chemistry** (5th Ed.), Wiley-India student edition
6. S. Mukerjee, 2007, **Mechanism and Structure in Organic Chemistry** (3rd Ed.), MacMillan Publishers India Limited

PHYSICAL CHEMISTRY-I

Credits: 4 **I Year/I Semester**

Subject Code: MOC16104 **No. of lecture hours: 60**

Objectives

- To understand the thermodynamic properties of reactions.
- To study the nature of electrochemical cells and their applications
- To impart knowledge about the subatomic particles of matter.
- To acquire the knowledge of kinetic mechanism.
- To study the photochemical properties and their applications.

Outcome

- The student will be able to understand the theories of reaction rates and as well as their electrochemical, thermodynamical, photochemical aspects.

Unit-01: Thermodynamics-I — 12 hrs

- Brief review of concepts of I and II laws of thermodynamics, concept of entropy, entropy as a state function, calculation of entropy changes in various processes. — **2**
- Entropy changes in an ideal gas, entropy changes on mixing of ideal gases, entropy as a function of V and T & Entropy as a function of P and T. Entropy change in isolated systems- Clausius inequality, entropy change as criterion for spontaneity and equilibrium. — **3**
- Third law of thermodynamics: Evaluation of absolute entropies from heat capacity data for solids, liquids and gases, standard entropies and entropy changes of chemical reactions. — **1**
- Helmholtz and Gibbs free energies (A and G), A and G as a criterion for equilibrium and spontaneity, physical significance of A and G, driving force for chemical reactions- relative signs of ΔH and ΔS. — **2**
- Thermodynamic relations: Gibbs equations, Maxwell relations, temperature dependence of G. Gibbs- Helmholtz equation. — **1**
- Chemical potential: Gibbs equations for non-equilibrium systems. Material equilibrium, phase equilibrium, Clapeyron equation and Clausius-Clapeyron equation. — **1**
- Conditions for equilibrium in a closed system, chemical potential of ideal gases, ideal-gas reaction equlibrium-derivation of equilibrium constant, temperature dependence of equilibrium constant-the van't Hoff equation. — **2**

Unit-02: Electrochemistry-I — 12 hrs

- Electrochemical Cells: Derivation of Nernst equation–problems, chemical and concentration cells (with and without transference), liquid junction potential (LJP)–derivation, its determination and elimination**.** — **3**
- Applications of EMF measurements: Solubility product, potentiometric titrations, determination of transport numbers, equilibrium constant measurements. — **2**
- Decomposition potential and its significance, Electrode polarization: its causes and elimination, concentration over potential. — **2**
- Amperometric titrations: Principle, Instrumentation and applications of — **2**

amperometric titrations, determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other substances.

- Cyclic voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms, Application: Cyclic voltammetric study of insecticide parathion. **3**

Unit -03: Quantum Chemistry- I **12 hrs**

- Black body radiation-Planck's concept of quantization-Planck's equation, average energy of an oscillator (derivation not required). **2**
- Wave particle duality and uncertain principle-significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schrodinger wave equation.**2hrs** **2**
- Operator**s**-operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. Operators ∇ and ∇^2. **2**
- Eigen functions and eigenvalues. Degeneracy. Linear combination of eigen functions of an operator. Well behaved functions. Normalized and orthogonal functions. **2**
- Postulates of quantum mechanics. Physical interpretation of wave function. Observables and operators. Measurability of operators. Average values of observables. **2**
- The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation. **2**

Unit-04: Chemical Kinetics **12 hrs**

- Theories of reaction rates: Collision theory, steric factor, transition state theory, reaction coordinate, activated complex and the transition state, thermodynamic formulation of transition state theory, activation parameters and their significance, the Eyring equation, unimolecular reactions and Lindemann's theory. **4**
- Complex reactions: Opposing reactions, parallel reactions and consecutive reactions (all first order type), chain reactions-general characteristics, steady state treatment example: H_2-Br_2 reaction, derivation of rate law. **4**
- Effect of structure on reactivity-linear free energy relationships, Hammett and Taft equations-substituent (σ and σ^*) and reaction constant (ρ and ρ^*) with examples, deviations from Hammett correlations, reasons-change of mechanism, resonance interaction, Taft four parameter equation, correlations for nucleophilic reactions. **4**

Unit -05: Photochemistry **12 hrs**

- Electronic transitions in molecules, Franck Condon principle, electronically excited molecules- singlet and triplet states, radiative life times of excited states-theoretical treatment, measured lifetimes. **3**
- Quantum yield and its determination, Actinomety: Ferrioxalate and Uranyl oxalate actinometers-problems. Derivation of fluorescence and phosphorescence quantum yields, E-type delayed fluorescence- evaluation of triplet energy splitting (ΔE_{ST}). **3**
- Photo physical processes, photo physical kinetics of unimolecular reactions, calculation of rate constants of various photo physical processes-problems, state diagrams. **2**
- Photochemical primary processes. Types of photochemical reactions- electron **2**

transfer, photo dissociation, addition, abstraction, oxidation and isomerization reactions with examples.

- Effect of light intensity on rates of photochemical reactions, photosensitization, quenching, Stern-Volmer equation. **1**
- Experimental set up of a photochemical reaction, introduction to fast reactions: Principle of flash photolysis. **1**

References:

Unit-01:

1. Peter Atkins and Julio de Paula, **Atkin's Physical Chemistry**, Oxford University press
2. Ira N. Levine, McGraw Hill, **Physical Chemistry**,
3. D. A. McQuarrie and J. D. Simon, **Physical Chemistry-A Molecular approach**, Viva Books Pvt. Ltd
4. D.A. McQuarrie and J.D. Simon, **Molecular Thermodynamics**, University Science Books

Unit-02:

5. S. Glasstone, **Introduction to Electrochemistry**.
6. J. O. M. Bockris & A. K. N. Reddy, Plenum, **Modern Electrochemistry**
7. Samuel H. Maron and Carl F. Prutton, **Principles of physical chemistry**, Oxford& IBH

Unit-03:

8. Ira N. Levine, Prentice Hall, **Quantum Chemistry**,
9. A. K. Chandra, **Introduction to Quantum Chemistry**, Tata McGraw Hill
10. R.K. Prasad Quantum Chemistry, New Age Publisher, 2010.

Unit-04:

11. Rajaraman and J. Kuriacose, **Kinetics and Mechanism of Chemical Transformations**, J McMillan
12. K.J. Laidler, **Chemical Kinetics**, McGraw Hill
13. J. H. Espenson, **Chemical Kinetics and Reaction Mechanisms**, McGraw Hill
14. Samuel H. Maron and Carl F. Prutton, **Principles of physical chemistry**, Oxford& IBH
15. Howard Maskill, **The Physical Basis of Organic Chemistry**, Oxford University Press (New York)
16. N. S. Isaacs, **Physical Organic Chemistry**, ELBS

Unit-05:

17. K. K. Rohtagi-Mukherji, **Fundamentals of Photochemistry**, Wiley-Eastern
18. N. J. Turro, **Molecular Photochemistry**, Benjamin
19. R. P. Kundall and A. Gilbert, **Photochemistry**, Thomson Nelson
20. A. Gilbert and J. Baggott, **Essentials of Molecular Photochemistry**, Blackwell Scientific Publications.
21. J. M. Coxon and B. Halton, **Organic Photochemistry**, Cambridge University press.
22. A. Cox and T. J. Kemp. **Introductory Photochemistry**, McGraw-Hill, London

ANALYTICAL TECHNIQUES AND SPECTROSCOPY-I

Credits: 4 **I Year/I Semester**

Subject Code: MOC16105 **No. of lecture hours: 60**

Objectives

- To acquire knowledge of chromatographic techniques.
- To gain knowledge of various spectroscopic techniques and their applications.

Outcome

- The student will learn about the various chromatographic and spectroscopic techniques.

Unit -01: Chromatography Techniques-I — 12 hrs

- Introduction to Chromatography and its classification. Gas Chromatography: Principle, Gas-Solid (GC, Adsorption) and Gas – Liquid (GLC, partition) chromatography. — **3**
- Performing GC, separations & Instrumentation: Stationary phases, carrier gases, retention indices, detectors (TCD, FID, and NPD). Temperature selection and quantitative measurements. Applications of GC- Analysis of Gasoline, separation of basic drugs, separation of free fatty acids from milk. — **4**
- High Performance Liquid Chromatography (HPLC): Principles, stationary phases, equipment, normal phase (NPC) and reverse-phase chromatography (RPC), solvents and columns for HPLC. Introduction to fast liquid chromatography. Applications of HPLC-Drug analysis (Antibiotics), Analysis of food products. — **4**
- Introduction to Ion Exchange Chromatography: Principles, cation and anion exchange resins and applications. — **1**

Unit- 02: NMR Spectroscopy-I — 12 hrs

- Magnetic properties of nuclei, principles of NMR. Instrumentation, CW and FT NMR. — **2**
- Equivalent and non-equivalent protons, enantiotopic and diastereotopic protons. Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, signal integration. — **4**
- Spin-spin coupling: vicinal-Karplus equation, geminal, long range and virtual coupling, coupling constants and factors affecting coupling constants. — **2**
- Applications of ^{1}H NMR spectroscopy: Structure determination, reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions). *E*, *Z*-isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange process, C-N rotation. — **4**

Unit-03: Rotational and Vibrational spectroscopy — 12 hrs

- **Rotational (Microwave) Spectroscopy:** Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy levels. Selection rules (derivation not required). — **2**
- Calculation of bond lengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer. — **1**

- **Vibrational Spectroscopy:** Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation of force constant from vibrational frequency. **1**
- Anharmonic nature of vibrations. Fundamental bands, overtones and hot bands, Fermi resonance. **1**
- Vibration-rotation spectra diatomic molecules. Vibrations of poly atomic molecules. Normal modes of vibration, concept of group frequencies. **1**
- Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding. **3**
- Applications of IR spectroscopy to the study of metal-ligand bonding modes involving monodentate and bidentate ligands. IR spectra of coordinated NO_3^- and SO_4^{2-} ions. **1**
- **Raman Spectroscopy**- Quantum theory of Raman Effect, Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra. **2**

Unit- 04: Electronic spectroscopy **12 hrs**

- Electronic spectra: Elementary energy levels of molecules. Selection rules for electronic spectra, types of electronic transitions in molecules. **2**
- Woodward-Fieser rules for chromophores: Conjugated dienes, trienes, unsaturated carbonyl compounds, benzene, and its derivatives, poly nuclear aromatic hydrocarbons, calculation of λ_{max}. **6**
- Solvent and structural influences on absorption maxima, stereo chemical factors. Cis-trans isomers, and cross conjugation. **2**
- Quantitative applications of electronic spectroscopy, dissociation constant of a weak acid, Charge transfer spectra. **2**

Unit -05: ESR Spectroscopy **12 hrs**

- Introduction, principle, instrumentation, selection rules. **2**
- Interpretation of Lande's factor 'g' in cubic, axial and rhombohedral geometry. **2**
- Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. **2**
- Zero field splitting, Kramer's degeneracy and quadrupolar interactions. **2**
- Study of free radicals and transition metal complexes. **2**
- Study of free radicals and evidence for covalency in complexes, ex: Cu(II) Bis-salcylaldimine, Bis-acetyl acetanato vanadyl(II) and hexa chloroiridium (IV) complexes. 2

References:

Unit 01:

1. Sane and Joshi, 1999, **Electro analytical Chemistry theory and applications,** Quest Publications.
2. Raymond PW Scott, **Techniques and practices of Chromatography,** Marcel Dekker, Inc. New York.
3. WMA Neissen& J V Greef, **Liquid Chromatography- Mass spectrometry Principles & Applications,** Marcel Dekker, Inc. New York.
4. Raymond PW Scott, 1988, **Introduction to analytical Gas Chromatography** (2nd Ed.), Marcel Dekker, Inc. New York

Unit 02, 03 & 04:

5. Banwell and Mc Cash, 1966, **Fundamentals of Molecular Spectroscopy,** McGraw-Hill.
6. G. M. Barrow, 1962, **Introduction to Molecular Spectroscopy**, McGraw-Hill.
7. J. R. Dyer, 1965, **Absorption Spectroscopy of Organic Compounds,** Prentice-Hall, Englewood Cliffs, N. J.
8. William Kemp, 2008, **Organic Spectroscopy** (3rd Ed.), Palgrave.
9. Pavia, 2004, **Introduction to organic spectroscopy** (3rd Ed.), Thomson
10. Jagmohan, 2010, **Organic Spectroscopy, Principles and Applications** (2ndEd.), Narosa Publication House Pvt. Ltd.

Unit 05:

11. Skoog, Holler and Nieman, Harcourt, 1998, **Principles of Instrumental analysis**, Asia PTE Ltd.
12. Skoog, West, Holler and Crouch, 2000, **Analytical Chemistry-An Introduction,** Saunders College Publishing.
13. Skoog and Leary, **Prinicples of Instrumental Analysis**, Saunders College Publishing.

INORGANIC CHEMISTRY PRACTICALS-I

Credits: 3 **I Year/I Semester**

Subject Code: MOC16151 **No. of hours/ week: 6 hrs**

Objectives

- To synthesise inorganic complexes.
- To understand the techniques involved in the preparation of standard solutions, standardization and estimations of metal ions.

Outcome

- The student will be able to synthesize various inorganic complexes and their estimations.

Calibrations:

- Calibration of weights.
- Calibration of pipettes.
- Calibration of standard flasks.
- Calibration of burette.

EDTA Back-titrations:

- Estimation of Ni^{2+}.
- Estimation of Al^{3+}.

EDTA Substitution titrations:

- Estimation of Ca^{2+}.

Preparation of complexes:

- Hexaammine nickel (II) chloride.
- Tris (acetylacetanato) manganese.
- Tris (ethylenediamine) nickel (II) thiosulphate.
- Mercury tetrathiocyanatocobaltate (II).
- Pentaammine (chloro) cobalt (III) chloride
- Potassium dioxalato Cuprate(II) dihydrate

Preparation of complexes and calculation of % purity:

- Tetrammine Copper (II)sulphate and estimation of NH_3 and calculation of % purity.

Redox Titrations

- Estimation of Ferrocyanide and Ferricyanide in a mixture

References:

1. A. I.Vogel, **Text book of Quantitative Inorganic Analysis** (3^{rd} Ed.), ELBS 1969.
2. Jeffery et.al, **Vogel's text book of Quantitative Inorganic analysis** (4^{th} Ed.), ELBS 1988.
3. Jeffery et.al, **Vogel's text book of Quantitative Inorganic analysis** (5^{th} Ed.), ELBS 1989.
4. J. Mendham et.al, **Vogel's text book of Quantitative Inorganic Analysis** (6^{th} Ed.), Pearson education Ltd., 2000.
5. G. Marr and R. W. Rockett, 1972, **Practical Inorganic chemistry**.
6. Mounir A. Malati, 1999, **Experimental Inorganic/Physical Chemistry–An Investigative integrated approach to Practical Project work**.

ORGANIC CHEMISTRY PRACTICALS-I

Credits: 3 **I Year/I Semester**

Subject Code: MOC16152 **No. of hours/week: 6 hrs**

Objectives

- To synthesise one-step organic compounds.
- To apply knowledge of Thin Layer Chromatography

Outcome

- The student will develop the skill to carry out the organic synthesis using TLC analysis

Synthesis of the following compounds:

p-Bromoacetanilide, *p*-Bromoaniline, 2,4,6-tribromoaniline, 1,3,5-tribromobenzene, tetrahydrocarbazole, 7-hydroxy-4-methyl coumarin, m-dinitrobenzene, hippuric acid, anthracene-maleic anhydride adduct, phthalimide.

Thin layer chromatography:

Determination of purity of a given sample, monitoring the progress of chemical reactions and identification of unknown organic compounds by comparing the R_f values of known standards and column chromatographic separations.

Demonstration experiment:

Synthesis of organic compounds by the use of microwave oven (any 2 examples)

References:

1. A. I. Vogel, 1989, **Text book of practical organic chemistry** (5^{th} Ed.).
2. F. G. Mann and B.C. 1990, **Saunders, Text book of practical organic chemistry** (5^{th} Ed.).

PHYSICAL CHEMISTRY PRACTICALS-I

Credits: 3 **Semester-I**

Subject Code: MOC16153 **No. of hours/week: 6 hrs**

Objective

- To apply the knowledge of various electro analytical techniques in studying reactions

Outcome

- The student will learn about various electroanalytical techniques.

Physical properties:

- Determination of viscosity of liquids

Distribution:

- Distribution of iodine between n-Hexane and water
- Distribution of I_2 between n-Hexane and aq.KI solution- calculation of equilibrium constant.

Chemical kinetics:

- Acid-catalyzed hydrolysis of methyl acetate
- Peroxydisulphate- I^- reaction (overall order)
- Effect of ionic strength on reaction rate

Conductometry:

- Titration of strong acid vs strong base
- Titration of weak acid vs strong base
- Determination of cell constant
- Determination of dissociation constant of a weak acid

Potentiometry:

- Titration of strong acid vs strong base
- Titration of weak acid vs strong base
- Titration of dibasic acid vs strong base
- Determination of single electrode potential

Polarimetry:

- Determination of specific rotation of sucrose, glucose
- Acid-catalyzed hydrolysis of sucrose (inversion of sucrose)

Adsorption and others:

- Adsorption of acetic acid on animal charcoal or silica gel
- Determination of critical solution temperature of phenol-water system
- Effect of added electrolyte on the CST of phenol-water system

References:

1. Text book of senior practical physical chemistry by B.D. Khosla.
2. Mounir A. Malati, 1999, **Experimental Inorganic/Physical Chemistry– An Investigative integrated approach to Practical Project work**.
3. J.B. Jadav **Advance Physical Practical Chemistry,** Krishna Publisher
4. A.K. Nad, B. Mahapatra and A. Ghoshal **A. Advance Course in Practical Chemistry**

VALUE EDUCATION & PERSONALITY DEVELOPMENT (THEORY)

Credits : 2 **I Year / Semester II**
Subject code : MOC16201 **No. of lecture hours: 30**

Objective

- To emphasize the importance of human values and inculcating them for the betterment of the society.

Outcome

- The student will learn about the human values and professional ethics.

UNIT- I **No of hours: 6**
INTRODUCTION TO ETHICS

- Reasons to have Ethics for Life 1
- Accepted Norms and Counter Values 1
- Happiness as life Goal 2
- Human Context-self and another 2

UNIT-II **No of hours: 6**
TOWARDS A NEW SOCIETY

- What is true society 1
- Moral problem of the society 1
- Social desire, social fear, social satence, social indifference 1
- Values revealed and lived in various religions-practicing religious harmony 2
- Eradication of social evil-towards a new society 1

UNIT-III **No of hours: 6**
GENDER SENSITIZATION

- Why we study it? 1
- Socialization-making women and men 1
- Being together as equals-through the lens of gender 1
- Knowledge through the lens of gender 1
- Gender spectrum-beyond the binary 1
- Just relationship-being together as equals 1

UNIT-IV **No of hours: 6**
PROFESSIONAL ETHICS

- Ethics, Professional Ethics, Environmental Ethics 1
- Ethical Situation, Current Ethical Issues 1
- Values, Policies and Organisation Culture 2
- Moral Situation, Rights and Duties, Codes of Ethics, Their Limitation 2

WORK SHEET (1): Self Estimation

UNIT-V **No of hours: 6**

ETHICS IN SCIENCE

- Professional Research in Academia and Industry, Scientific fraud 1
- Plagiarisum, Conflict of Inters 1
- Student-Advisor relationship, Intelectual property and Patents 2
- Acountability and Institutional Practices 2

TEXT BOOKS:

1. *Human Values - Development Programme - AIACHE*
2. *In Harmony*
3. S.S. Dara and D.D. Mishra 2010. **Environmental Chemistry and Pollution Control** New Delhi: *S. Chand Publisher.*
4. Jeffery Kovac, Ethics in Science, **Accountability in Research** *22*, 312, **2015**.
5. A.Suneetha, B.Uma, D. Vasanta, M. Rama, N. Vasundha, A. Raheed, G**,** Shamala, D. Sreenivas and S. Tharu 201. **Towards a World of Equals: A Bilingual Text on Gender**. Hyderabad: Telugu Akademi

INORGANIC CHEMISTRY-II

Credits: 4 **I Year / II Semester**

Subject Code: MOC16202 **No. of lecture hours: 60**

Objectives

- To impart knowledge of co-ordinate complexes, their reaction mechanisms and metal clusters
- To acquire the knowledge of special symmetry groups and assign the same to the molecules.
- To understand the role of metal ions in biological systems.

Outcome

- The student will be familiar with higher symmetry point groups and role of metal ions in biological system.

Unit 06: Bonding in metal complexes- II

Total=12 hrs

- Free ion terms and Energy levels: Configurations, Terms, States and Microstates. **3 hrs**
- Formula for the calculation of Microstates p^n and d^n configurations: L-S (Russel-Saunders) coupling scheme, j-j coupling scheme. **3 hrs**
- Determination of terms for various p^n and d^n configurations of metal ins. Hole formalism, Energy ordering of terms (Hund's rules). Inter electron repulsion parameters (Racah parameters), Spin-Orbital coupling parameters. **3 hrs**
- Effect of weak cubic crystal fields on S, P, D and F terms- Orgel diagrams. Application of electronic spectra of metal complexes-$3d^1$ to $3d^9$ hexaaquo metal complexes. **3 hrs**

Unit 07: Symmetry of molecules

12 hrs

- Molecules of special Symmetry: Linear or Infinite groups, Molecules containing multiple higher order axis T, Th, Td, O, O_h, I_h, K_h . **4**
- Excersises on point groups, descent in symmetry of molecules with substitution. **2**
- Symmetry and stereo isomerism: Symmetry and dipole moment, symmetry criteria for optical activity, symmetry restrictions on dipole moment. **4**
- Fullerenes: Structure and symmetry of fullerenes. **2**

12 hrs

Unit- 08: Reaction Mechanism-II

- Ligand substitution reactions in square planar complexes: Mechanism of substitution in square planar complexes, trans-effect, Grienberg's polarization theory and π - bonding theory, applications of Trans-effect in synthesis of Pt (II) complexes. **4**
- Electron transfer reactions (or Oxidation-Reduction) in Coordination compounds: Mechanism of One-electron transfer reactions: Atom or (group) Transfer or Inner Spheres Mechanism, Direct electron transfer or Outer sphere mechanism. Complementary & non complementary reactions Marcus Hush theory. **3**
- Nature of bridging ligands. Distinguish between, outer sphere & inner sphere electron transfer reaction mechanism. **3**
- Reaction pathways in organometallic complexes. Oxidative addition reductive elimination insertion reactions **2**

Unit 09: Metal clusters

12 hrs

- Boranes: Synthesis of neutral boron hydrides, polyhedral boranes anions and **3**

dianions, structure of polyhedral boranes: nido, arachno and closo frame works, Polyhydral skeletal electron pair theory and total electron count theory, Wade's rules and polyhedral geometries.

- Carbonyl clusters: Factors favouring metal-metal bonding **1**
- Classification of clusters: Low nuclearity clusters: M_3 and M_4 clusters. Structural patterns in $M_3(CO)_{12}$ [M=Fe, Ru, Os] and $M_4(CO)_{12}$ [M=Co, Rh, Ir] clusters. Relative stability of bridging and nonbridging structures. **2 hrs**
- High Nuclearity clusters: M_5, M_6, M_7, M_8 and M_{10} clusters. Capping rule. **1 hr**
- Structural patterns in $[Os_6(CO)_{18}]^{2-}$, $[Rh_6(CO)_{16}]$, $[Os_7(CO)_{21}]$, $[Rh_7(CO)_{16}]^{3-}$, $[Os_8(CO)_{22}]^{2-}$, $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_5(CO)_{12}]^{2-}$. **2 hrs**
- Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems: Edge sharing Bioctahedra, Face sharing Bioctahedra, Tetragonal prismatic and Trigonalantiprismatic structures. **2**
- Structure and bonding in $[Re_2Cl_8]^{2-}$ and Octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$, Trinuclear halides of Re (III). **1**

Unit 10: Bio Coordination Chemistry **12 hrs**

- Metal ions in biological systems: Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects. **2**
- Oxygen transport and storage: Haemoglobin and Myoglobin: Geometric, electronic and magnetic aspects of dioxygen binding, oxygen adsorption isotherms and cooperativity in haemoglobin and its physiological significance. Role of globin chain, haemerythrin and haemocyanin. **4**
- Structure of deoxy forms, oxygen binding, geometric, electronic and magnetic aspects. Comparison of haemerythrin and haemocyanin with haemoglobin. **3**

- Photosynthesis: Structural aspects of chlorophyll. Photo system I and Photo system II. **1**
- Vitamin B_6 model systems: Structures vitamin B_6. Reaction mechanisms of transamination, Trans aldonation and decarboxylation **2**

References:

Unit 05:

1. J. E. Huheey, K. A. Keiter and R. L. Keiter, 1993, **Inorganic Chemistry** (4th Ed.), Harper Cottens College Publications.

Unit 06:

2. K.Veera Reddy, 2005. **Metal ions in Reaction Mechanisms** (1st Ed.), Golgotia Publications (P) Ltd.
3. Richard A Henderson, 1993, **Mechanisms of Reactions in Transition Metal Sites,** Oxford Science Publications, London.
4. F. Basolo and R. G. Pearson, 1967, **Inorganic Reaction Mechanisms** (2nd Ed.), Wiley, New York.

Unit 07:

5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 1999, **Advanced Inorganic Chemistry** (6th Edition), Wiley Inter science, New York.
6. G. L. Eichorn, 1982, **Inorganic Biochemistry** (Vol. 1)., Elsevier
7. Keith F. Purcell and John C. Kotz, 1977, **Inorganic Chemistry**, Holt-Saunders International Editions, London.

Unit 08:

8. I. Bertini, H. B. Gray, S. J. Lippard and S J. Valentine, 1998, **Bioinorganic Chemistry** (1st Ed.), Viva Low- Priced Student Edition, New Delhi.
9. W. Kain and B. Schwederski, 1999, **Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life**, John Wiley and Sons, NY.
10. Keith F. Purcell and John C. Kotz, 1977, **Inorganic Chemistry**, Holt-Saunders International Editions, London.

ORGANIC CHEMISTRY-II

Credits: 4 **I Year / II Semester**

Subject Code: MOC16203 **No. of lecture hours: 6**

Objectives

- To understand the mechanisms in organic reactions involving aromatic systems.
- To acquire knowledge of pericyclic and photochemical reactions.
- To have an understanding of the applications of various reagents in organic reactions.

Outcome

- The student will learn to apply the knowledge of various reagents in the different reaction and have an understanding of pericyclic and photochemical reactions.

Unit- 06: Reaction Mechanism-II **12 hrs**

- Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: S_N1 (Ar), S_N2 (Ar), and benzyne mechanisms. Definition and types of ambident nucleophiles. **4**
- Neighboring group participation: Criteria for determining the participation of neighboring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. **4**
- Neighboring group participation involving halogens, oxygen, sulphur, nitrogen, aryl, cycloalkyl groups,σ and π- bonds, and non-classical carbocations. **4 s**

Unit-07: Pericyclic Reactions-I **12 hrs**

- Introduction, Classification of pericyclic reactions, 4n, 4n+2 systems and examples. **1**
- Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in 4n and 4n+2 systems. **2**
- Cycloaddition reactions: suprafacial and antara facial additions. 4n and 4n+2 cycloadditions. Stereochemical aspects in supra-supra, supra-antara, antara-supra and antara-antara 4n and 4n+2 cycloadditions, Diels Alder reaction *(endo-exo)-stereoselectivity*. **4**
- Sigmatropic reactions [i, j] shifts- suprafacial and antarafacial shifts, Cope, Aza-Cope and Claisen rearrangement reactions. **3**
- Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical. **2**

Unit-08: Pericyclic Reactions-II **12 hrs**

Theories involved in understanding pericyclic reactions: **4**

- Introduction to Aromatic Transition state Theory: Concept, Woodward- Hoffman se1ection rules for electrocyclic reactions, cycloaddition and sigmatropic reactions based on ATS aromatic transition state (Huckel-Mobius) approach.
- Frontier Molecular Orbital Theory: Concept, Woodward- Hoffman selection rules for electrocyclic, cycloaddition, and sigmatropic reactions based on FMO approach. **4**
- Conservation of Molecular Orbitals Theory: Construction of correlation diagram for 4n & 4n+2 electrocyclic reactions and cycloaddition ($\pi^2s+\pi^2s$ and $\pi^4s+\pi^2s$) systems. **4**

Unit-09: Photochemistry **12 hrs**

- Photochemistry of π-π* transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. **2**
- Rearrangements: di-π methane, oxa di-π methane rearrangement. **2**

Photoisomerisation of benzene.

- Photochemistry of n-π* transitions: Excited states of carbonyl compounds. Homolytic cleavage of α- bond Norrish type I reaction in acyclic and cyclic ketones. **3**

- Intermolecular abstraction of hydrogen: photoreduction. **1**
- Intramolecular abstraction of hydrogen: Norrish type II reaction. **2**
- Paterno-Buchi reaction. **1**
- Photochemistry of nitrites: Barton reaction. **1**

Unit-10: Oxidation and Reduction Reagents

12 hrs

Oxidation Reagents:

- Alcohols to carbonyls: CrVI oxidants-(CrO3, Jones reagent, PCC, PDC) **2**
- Introduction to IBX, DMP. **1**
- Swern oxidation, Silver Carbonate. **1**
- Oxidation of allylic and benzylic C-H bonds: NBS, DDQ and SeO_2. **2**

Reduction reagents: **1**

- Catalytic hydrogenation: Homogenous and heterogeneous catalytic reduction.
- Dissolving metal reductions: Birch reduction. **1**
- Nucleophilic metal hydrides: $LiAlH_4$, $NaBH_4$ and their modifications (alkoxy aluminates, DIBAL-H, sodium cyanoborohydride) **2**
- Electrophilic metal hydrides: BH_3. **1**
- Hydrogenolysis: use of tri-n-butyl tin hydride. **1**

References:

Unit 06:

1. Jerry March, 1992, **Advanced Organic Chemistry** (5th Ed.), Wiley-India student edition
2. S. Mukerjee,2007, **Mechanism and Structure in Organic Chemistry** (3rd Ed.), MacMillan Publishers India Limited
3. I. L. Finar, 1963, **Organic chemistry** (4th Ed.), Vol. I and II, Longmans
4. D. H. R. Barton and W. D. Ollis, 1978, **Comprehensive organic chemistry**, Vol.5.

Unit 07& 08:

5. Woodward and Hoffmann, 1971,**Conservation of Orbital Symmetry Available** as e-book.
6. Gilchrist and Storr, 1979, **Organic Reactions and Orbital Symmetry**, Cambridge University Press.
7. J.Singh, 2006, **Photochemistry and Pericyclic reactions** (2nd Ed.), New Age International publishers.
8. Lehr and Merchand, 1972. **Pericyclic Reactions— a problem solving approaches**, Academic Press: New York.

Unit 09:

9. Depuy and Chapman, 1988. **Molecular Reactions and Photo chemistry**, Prentice Hall of India Pvt. Ltd.
10. Nicholas Turro and others, 2009, **Principles of Molecular Photochemistry-An Introduction.** University Science Books.
11. D Coyle, 1998. **Organic Photochemistry** (4th Ed.), John Wiley &Sons.

Unit 10:

12. W Carruthers, 2004, **Modern methods of organic synthesis** (4th Ed.), Cambridge University Press.

13. Jagadamba Singh and L. D. S. Yadav, 2011, **Organic synthesis**, Pragathi Prakasan publications.
14. R K Meckie, D M Smith & R A Atken, 1990, **Guide book to organic synthesis** (2nd Ed.), Longman.
15. Michael B Smith, 1994, **Organic synthesis**, MacGrawHill International Editions.
16. Fieser & Fieser, 2007, reprint, **Reagents for organic synthesis**, Vol 1-11, Wiley India.
17. C Willis and M Willis, 1995. **Organic Synthesis**, Oxford University press

PHYSICAL CHEMISTRY-II

Credits: 4 **I Year / II Semester**

Subject Code: MOC16204 **No. of lecture hours: 60**

Objectives

- To understand the thermodynamic properties of reactions.
- To study the nature of electrochemical cells and their applications
- To impart knowledge about the subatomic particles of matter.
- To acquire the knowledge of kinetic mechanism.
- To understand the concepts of solid state chemistry.

Outcome

- The student will have a further understanding of the kinetics of the reactions along with their thermodynamic, electrochemical and solid state properties.

Unit -06: Thermodynamics-II **12 hrs**

- Solutions: Specifying the Solution composition, partial molar properties-significance, relation between solution volume and partial molar volume. Measurement of partial molar volumes: slope and intercept methods **3**
- The chemical potential, variation of chemical potential with T and P, Gibbs-Duhem equation-derivation and significance. **2**
- Ideal solutions: Thermodynamic properties of ideal solutions, mixing quantities, vapour pressure-Raoult's law. Thermodynamic properties of ideally dilute solutions vapour pressure- Henry's law. **2**
- Non ideal systems: Concept of fugacity, fugacity coefficient, determination of fugacity. Non ideal solutions: Activities and activity coefficients, standard-state conventions for non-ideal solutions, determination of activity coefficients from vapour pressure measurements, activity coefficients of nonvolatile solutes using Gibbs-Duhem equation. **4**
- Multi component phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation. **1**

Unit -07: Electrochemistry-II **12 hrs**

- Types and Classification of Electro analytical Methods. **2**
- Potentiometry: Types of electrodes, Hydrogen gas, Calomel, Quinhydrone and glass electrodes. Determination of pH. Potentiometric titration of redox reaction. **3**
- Conductometry: Definition of terms: Conductivity, specific conductivity, cell constant, mobility of ions. Conductometric titration of weak acid against strong base. **3**
- D.C Polarography: Two and Three electrode assemblies. Dropping mercury electrode. Instrumentation. **2**
- Types of Currents: Residual, Migration, Limiting. Types of limiting Currents: Adsorption, Diffusion, Kinetic. **2**

Unit -08: Quantum chemistry-II **12 hrs**

- **Theorems of quantum mechanics**. Real nature of the Eigen values of a Hermitian operator-significance. Orthogonal nature of the Eigen values of a Hermitian **3**

operator-significance of orthogonality. Expansion of function in terms of eigenvalues. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

- Particle in a box- one dimensional and three dimensional. **1**
- Plots of ψ and ψ^2-discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles. **1**
- Calculations using wave functions of the particle in a box-orthogonality, measurability of energy, position and momentum, average values and probabilities. **2**
- Application to the spectra of conjugated molecules. **2**
- Cartesian, Polar and spherical polar coordinates and their interrelations. Schrodinger equation for the hydrogen atom- separation into three equations. **3**

Unit -09: Quantum chemistry-III **12 hrs**

- Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. **2**
- The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour pots and boundary diagrams. **2**
- Many electron systems. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. **2**
- Examples of variational calculations. Particle in a box. Construction of trial functions by the method of linear combinations. Variation parameters. Secular equations and secular determinant. **2**
- Bonding in molecules. Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion. The variational integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram. **2**
- The MO wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required). The MO wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required). **2**

Unit -10: Solid state chemistry **12 hrs**

- Magnetic properties of solids- classification of magnetic materials, Magnetic susceptibility, Langevin theory of diamagnetism & Weiss theory of paramagnetism. **2**
- **Electronic properties of metals, insulators and semiconductors**: Electronic structure of solids, Band theory- band structure of metals, insulators and semiconductors. **2**
- Electrons, holes and excitons, the temperature dependence of conductivity of extrinsic semiconductors, photo conductivity and photovoltaic effect-*p-n* junctions. **2**
- **Superconductivity*:*** Occurrence of superconductivity, destruction of superconductivity by magnetic fields-Meisner effect, theories of super conductivity-BCS theory. **3**
- **High temperature superconductors*:*** Structure of defect pyrovskites. High T_c super conductivity in cuprates, phase diagram of Y-Ba-Cu-O system, crystal structure of $YBa_2Cu_3\ O_{7-x}$, preparation of 1-2-3 materials, origin of high T_c superconductivity. **3**

References:

Unit 06:

1. Peter Atkins and Julio de Paula, **Atkin's Physical Chemistry**, Oxford University press

2. Ira N. Levine, **Physical Chemistry**, McGraw Hill
3. D. A. Mc Quarrie and J. D. Simon, **Physical Chemistry-A Molecular approach**, Viva Books Pvt. Ltd
4. D. A. Mc Quarrie and J. D. Simon, Molecular Thermodynamics, University Science Books

Unit 07:

5. Heyrovsky, 1966, **Principles of Polarography,** Publishing House of the Czechoslovak Academy of Sciences,
6. R. C. Kapoor., B. S. Agarwal, 1991, **Principles of Polarography,** Wiley.
7. C. Charlot, 1962, **Modern Electro analytical methods,** Elsevier Company.

Unit 08 & 09:

8. Ira N. Levine, **Quantum Chemistry**, Prentice Hall
9. A. K. Chandra, **Introduction to Quantum Chemistry**, Tata McGraw Hill

Unit 10:

10. Leonid V. Azaroff, **Introduction to Solids**, Tata McGraw Hill
11. D. K. Chakrabarthy, **Solid state Chemistry**, New Age International
12. A. R. West, **Solid state Chemistry and its applications**, Plenum.
13. H. V. Keer, **Principles of the SolidState**, New Age International

ANALYTICAL TECHNIQUES AND SPECTROSCOPY-II

Credits: 4 **I Year / II Semester**

Subject Code: MOC16205 **No. of lecture hours: 60**

Objectives

- To acquire knowledge of hyphenated techniques.
- To gain knowledge of various spectroscopic techniques and their applications.

Outcome

- The student will be familiar spectroscopic (NMR, PES, MSS) and hyphenated techniques.

Unit-06: Chromatography Techniques-II — Total=12 hrs

- **GC-MS:** Principle, instrumentation; interfaces, jet separators, mass analyzer, mass chromatogram with an example, applications. — **3 hr**
- **GC-FT-IR**: Instrumentation, principles and applications. — **3 hrs**
- **LC-MS**: Instrumentation, principles, interfaces and applications. — **3 hrs**
- **ICP-MS**: Instrumentation, principles, quantitative analysis and applications. — **3 hrs**

Unit- 07: NMR spectroscopy-II& ^{19}F NMR spectroscopy: — Total=12 hrs

- First order and non-first order spectra e.g., AX, AX_2, AX_3, A_2X_3, AMX and AB. — **3 hrs**
- Simplification of complex spectra: increased field strength, deuterium exchange, Lanthanide shift reagents and double resonance techniques. — **3 hrs**
- Nuclear Overhauser enhancement (NOE). — **1 hr**
- Study of aromaticity and fluxional molecules (eg.$[C_8H_8Ru(CO)_3]$, NMR of paramagnetic compounds: acetylacetone complexes. — **2 hrs**
- **^{19}F NMR spectroscopy**: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F, ^{1}H and ^{31}P: 2,2,2-trifluoro ethanol, 1,2-dichloro-1,1-difluoro ethane, 5-bromo-1,2,3-trifluoro benzene, BrF_5, SF_4, PF_5, ClF_3, IF_5. — **3 hrs**

Unit- 08: Mass spectrometry-I — Total=12 hrs

- Origin of mass spectrum, principles of EI mass spectrometer — **2 hrs**
- Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula and metastable ion peaks. — **4 hrs**
- Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Thermospray (TSI) ionization, and Matrix Assisted Laser Desorption Ionization (MALDI) methods. High resolution mass spectrometry. — **6 hrs**

Unit- 09: Mass spectrometry-II — Total=12 hrs

- Fragmentation pattern of organic compounds: cleavage of one, two or more bonds, β-cleavage, McLafferty rearrangement, retro Diels–Alder fragmentation, ortho effect, dehydration, dehydrohalogenation, decarboxylation and elimination of NO. Determination of molecular formula. — **8 hrs**
- Fragmentation of cycloalkanols, cycloalkanones and cyclo alkyl amines. — **2 hrs**
- Application of mass spectrometry to metal carbonyls. — **2**

Unit -10: Photoelectron Spectroscopy — 12 hrs

- Introduction, principle and instrumentation, types of Photoelectron Spectroscopy – UPS & XPS Binding Energies, Koopman's Theorem, Chemical Shifts. — **3**
- Photoelectron Spectra of Simple Molecules: N_2, O_2^- Vibrational Structure of PES — **3**

Bands, Potential energy curves.

- Interpretation of Vibrational spectral data for ionized (M^+) species, Prediction of Nature of Molecular Orbitals. **3**
- ESCA in qualitative analysis, Principles of Auger electron spectroscopy. **3**

References:

1. **Unit 06:** Sane and Joshi, 1999, **Electro analytical Chemistry theory and applications,** Quest Publications.
2. Raymond PW Scott, **Techniques and practices of Chromatography,** Marcel Dekker, Inc. New York.
3. WMA Neissen& J V Greef, **Liquid Chromatography- Mass spectrometry Principles & Applications,** Marcel Dekker, Inc. New York.
4. Raymond PW Scott, 1988, **Introduction to analytical Gas Chromatography** (2nd Ed.), Marcel Dekker, Inc. New York

Unit 07:

5. Jag Mohan, 2008, **Organic spectroscopy-Principles applications** (2nd Ed.), Narosa publications.
6. William Kemp, 2008, **Organic Spectroscopy** (3rd Ed.), Palgrave.
7. R.M. Silverstein and F.X. Webster, 1998, **Spectroscopic identification of organic compounds,** (6th Ed), Wiley.
8. William Kemp, 1988, **NMR-A multinuclear introduction** (3rd Ed.), MacMillan.
9. W. Dolbier, 2009, **Guide to Fluorine NMR for organic chemist** (1st Ed.), Wiley.

Unit 08 & Unit 09:

10. A. H. Beckett and J.B. Stenlake, 1988, **Practical Pharmaceutical Chemistry** (4th Ed.),WCIR, London
11. Robert Alexander Walker Johnstone, 1996, **Mass Spectrometry for Chemists and Biochemists** (2nd Ed.), Cambridge University Press.

Unit 10:

12. Skoog, Holler and Nieman, Harcourt, 1998, **Principles of Instrumental analysis**, Asia PTE Ltd.
13. Skoog, West, Holler and Crouch, 2000, **Analytical Chemistry-An Introduction,** Saunders College Publishing.
14. D. Beckerand D. Betteridge**,** 1972, **International series of Monographs, Vol. 53: Photoelectron Spectroscopy**

INORGANIC CHEMISTRY PRACTICALS-II

Credits: 3 **I Year / II Semester**

Subject Code: MOC16251 **No. of hours/week: 6**

Objectives

- To analyse the metal ions gravimetrically.
- Separation and analysis of mixture of complexes volumetrically and gravimetrically.

Outcome

- The student will learn to perform gravimetric and volumetric analysis of the inorganic complexes.

One component gravimetric estimations (Use of sintered glass crucible):

- Estimation of Zn^{2+}.
- Estimation of Ba^{2+}.

Analysis of Two component mixtures:

- Separation of Ni^{2+} and Cu^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+} (volumetric).
- Separation of Fe^{2+} and Mg^{2+} in a mixture and estimation of Fe^{2+} (gravimetric) and Mg^{2+} (volumetric).
- Separation of Al^{3+} and Fe^{3+} in a mixture and estimation of Al^{3+} (gravimetric) and Fe^{3+} (volumetric).
- Separation of Ag^{+} and Ca^{2+} in a mixture and estimation of Ag^{+} (gravimetric) and Ca^{2+} (volumetric).

Analysis of three component mixtures:

- Separation of (Fe^{2+} and Ni^{2+}) from Zinc (Zn^{2+}) in the given mixture and estimation of Zinc (Gravimetric).
- Separation of (Ni^{2+} and Cu^{2+}) from Mg^{2+} in the given mixture and estimation of Mg^{2+} (Gravimetric).

Ion exchange methods of analysis:

- Determination of capacity of an ion exchange resin.
  Separation of Zinc and Magnesium on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+}

References:

1. A. I. Vogel, 1969, **Text book of Quantitative Inorganic Analysis** (3rd Ed.), ELBS.
2. Jeffery et.al, 1988, **Vogel's text book of Quantitative Inorganic analysis** (4th Ed.), ELBS.
3. Jeffery et.al, 1989, **Vogel's text book of Quantitative Inorganic analysis** (5th Ed.), ELBS
4. J. Mendham et.al, 2000, **Vogel's text book of Quantitative Inorganic Analysis** (6th Ed.), Pearson education Ltd.

ORGANIC CHEMISTRY PRACTICALS-II

Credits: 3 **I Year / II Semester**

Subject Code: MOC16252 **No. of hours/week: 6**

Objectives

- To identify the given organic compound and assign its functional group qualitatively.
- To separate an organic mixture and apply systematic functional group analysis.

Outcome

- The student will be able to separate the mixture and analyze the organic functional groups present.

Identification of organic compounds systematic qualitative analysis:

- Physical data BP / MP, Ignition test, solubility classification, Extra elements-N, S & Halogens, (Lassagnine sodium fusion test)
- Functional groups tests, Preparation of crystalline derivative and determination of their mp's for atleast**4** compounds belonging to strong acid, weak acid, neutral, bases, carbohydrates & hydrocarbons.

Separation of two component mixtures by chemical methods and their identification by chemical reactions

- Separation by using solvent ether, dil hydrochloric acid, 5 % aqueous sodium bicarbonate and sodium hydroxide solutions.
- Checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives.

  A minimum of **6** mixtures should be separated and analyzed by these procedures.
  Following combinations can be given:
  Strong acid + Neutral including Hydrocarbons, Strong acid + Weak acid, Weakacid + Neutral including hydrocarbon, Base+hydrocarbon, Carbohydrate + weak acid, Carbohydrate+strong acid (other than p-nitrobenzoic acid)

References:

1. A .I. Vogel, 1989, **Text book of practical organic chemistry** (5^{th} Ed.).
2. F. G. Mann and B.C. 1990, **Saunders, Text book of practical organic chemistry** (5^{th} Ed.).

PHYSICAL CHEMISTRY PRACTICALS-II

Credits: 3 **I Year / II Semester**

Subject Code: MOC16253 **No. of hours/week: 6**

Objectives

- To apply the knowledge of various electro analytical techniques in studying reactions

Outcome

- The student will be able to perform various experiments involving different analytical techniques

Chemical Kinetics:

- Peroxydisulphide- iodide reaction: order w.r.t [I-] by isolation method
- Peroxydisulphide- iodide reaction: order w.r.t [$S_2O_8^{2-}$] by initial rate method
- Study of acetone-iodine reaction by spectrophotometry
  - i) Order w.r.t.[iodine]
  - ii) Order w.r.t. [acetone]

Conductometry:

- Titration of a mixture of strong and weak acids vs strong base
- Mixture of strong acid, weak acid and CuSO4 vs strong base
- Determination of the hydrolysis constant of aniline hydrochloride

Potentiometry:

- Titration of Fe^{+2}vs $Cr_2O_7^{-2}$ (redox titration)
- Titration of Cl^- vs Ag+ (precipitation titration)
- Determination of solubility product

pH metry:

- Calibration of a pH meter and measurement of pH of different solutions
- Preparation of phosphate buffers.
- Monobasic acids vs strong base.
- Dibasic acid vs strong base

Spectrophotometry:

- Estimation of Cu(II) using EDTA.
- Estimation of Fe(II) using 1,10-phenanthroline

Distribution:

- Distribution of iodine between Hexane and water
- Distribution of I_2 between Hexane and aq.KI solution- calculation of equilibrium constant.

References:

1. B. D. Khosla, **Text book of senior practical physical chemistry** R. Chand & Co. New Delhi
2. Mounir A. Malati, 1999, **Experimental Inorganic/Physical Chemistry–An Investigative integrated approach to Practical Project work**.
3. J.B. Jadav **Advance Physical Practical Chemistry,** Krishna Publisher
4. A.K. Nad, B. Mahapatra and A. Ghoshal **A. Advance Course in Practical Chemistry**