Rayat Shikshan Sanstha's

Karmaveer Bhaurao Patil College, Vashi, Navi Mumbai

Autonomous College

[University of Mumbai]

Syllabus for Approval

Sr. No.	Heading	Particulars
1	**Title of Course**	**M.Sc.-II Chemistry**
2	**Eligibility for Admission**	**B.Sc. Chemistry of any recognized University**
3	**Passing marks**	40%
4	**Ordinances/Regulations (if any)**	
5	**No. of Years / Semesters**	**One Year / Two Semesters**
6	**Level**	**P.G.**
7	**Pattern**	**Semester**
8	**Status**	**New (NEP)**
9	**To be implemented from Academic year**	**2024-2025**

AC - / / 2024

Item No-

Rayat Shikshan Sanstha's
KARMAVEER BHAURAO PATIL COLLEGE, VASHI.
NAVI MUMBAI
(AUTONOMOUS COLLEGE)
Sector-15- A, Vashi, Navi Mumbai - 400 703

Syllabus for M.Sc.- II In Chemistry

Program: M.Sc. Chemistry

Course: M.Sc. – II Chemistry

[NATIONAL EDUCATION POLICY (NEP 2020) with effect from the academic year 2024-2025]

Preamble of the Syllabus:

Master of Science (M.Sc.) in Chemistry is a post-graduation program of Department of Chemistry, Karmaveer Bhaurao Patil College Vashi, Navi Mumbai. The revised syllabus in Chemistry as per National Education Policy (NEP 2020) for **M. Sc. Part–II** program will be implemented from the academic year **2024-25.**

The systematic and planned curricula from these courses through the National Education Policy (NEP 2020) to be implemented would allow students to motivate and encourage learners to understand basic concepts in Chemistry and to understand the real world problems.

The learners are expected to enrich knowledge through thinking and reasoning abilities, numerical problem solving, hands-on activities, study tours, industrial visits and research projects etc.

The learners are expected to develop critical, analytical and reasoning abilities towards real world problems and become familiarize with the recent scientific and technological advancements.

Program Outcomes (POs):

PO-1	**Disciplinary Knowledge and Skills:** Acquire the comprehensive and in-depth knowledge of various subjects in sciences such as Chemistry, Chemistry, Mathematics, Microbiology, Bio-analytical Science, Computer Science, Data Science, Information Technology and disciplinary skills and ability to apply these skills in the field of science, technology and its allied branches.
PO-2	**Communication and Presentation Skills:** Develop various communication skills including presentation to express ideas evidently to achieve common goals of the organization.
PO-3	**Creativity and Critical Judgement:** Facilitate solutions to current issues based on investigations, evaluation and justification using evidence based approach.
PO-4	**Analytical Reasoning and Problem Solving:** Build critical and analytical attitude in handling the problems and situations.
PO-5	**Sense of Inquiry:** Curiously raise relevant questions based on highly developed ideas, scientific theories and its applications including research.
PO-6	**Use of Digital Technologies:** Use various digital technologies to explore information/data for business, scientific research and related purposes.
PO-7	**Research Skills:** Construct, collect, investigates, evaluate and interpret information/data relevant to science and technology to adapt, evolve and shape the future.
PO-8	**Application of Knowledge:** Develop scientific outlook to create consciousness against the social myths and blind faith.
PO-9	**Moral and Ethical Reasoning:** Imbibe ethical, moral and social values to develop virtues such as justice, generosity and charity as beneficial to individuals and society at large.
PO-10	**Leadership and Teamwork:** Work cooperatively and lead proactively to achieve the goals of the organization by implementing the plans and projects in various field-based situations related to science, technology and society at large.
PO-11	**Environment and Sustainability:** Create social awareness about environment and develop sustainability for betterment of future.
PO-12	**Lifelong Learning:** Realize that pursuit of knowledge is a lifelong activity and in combination with determined efforts, positive attitude and other qualities to lead a successful life.

Program Specific Outcomes (PSO)

PSO-1	**Scientific Problem solving skills:** Deep knowledge of the topic which can develop the problem solving skills using chemical principles.
PSO-2	**Analytical skills:** Develop analytical skills such as synthesizing, separating, characterizing chemical compounds and chemical reaction with the help of sophisticated instruments..
PSO-3	**Research skills:** Develop research skills through dissertation/Project work in different fields of chemistry such as organic, nanoscience, analytical, CHEsical etc.

SCHEME OF EXAMINATION FOR EACH SEMESTER

Continuous Internal Assessment: 40% (Unit Test-20 Marks & 10 Marks for- Assignment, Oral, Seminar, Presentation, Group Discussion, Participation in Conf / Sem / Workshop, Open Book Test, Visit to Research Institute etc)

Semester End Examination: 45 Marks (2 ½ hrs duration) will be as follows:

I.	**Theory:**	
	Each theory paper shall be of TWO and HALF Hour duration.	
	Each paper shall consist of FOUR questions. All questions are compulsory and will have internal options.	
	Q – I :	is from Unit – I (15 Marks)
	Q – II :	is from Unit – II (15 Marks)
	Q – III :	is from Unit – III (15 Marks) … for 3 Unit Courses
	Q – IV :	is from Unit – IV (15 Marks) … for 4 Unit Courses
II.	**Practicals:**	The External examination per practical course will be conducted as per the following scheme.

Sr. No.	**Particulars of External Practical Examination**	**Marks**
1	Practicals based on Course CHE501	25
2	Practicals based on Course CHE502	25
3	Practicals based on Course CHE503	50
4	Practicals based on Course CHE504A/ CHE504B	25
	TOTAL =	**125**

Syllabus for M.Sc. Part – II Chemistry (Theory & Practical)

Course Structure & Distribution of Credits

1. General:

M. Sc. in Chemistry Program consists of total 12 Core Courses (CC), 04 Discipline Specific Elective (DSE) Courses, spread over four semesters. In addition to these, Research Methodology Course of 4 credits in Sem-I, Internship of 4 credits in Sem – II), Project Dissertation of 4 credits each in Sem – III & Project Dissertation of 6 credits each in Sem IV are made compulsory for all the students. In Sem-III, 3 theory course (CC - 2 & DSE - 1) will be of 4 credits and 1 CC course will be of 6 credits in addition to research projects for 4 Credits. In Sem – IV, 4 theory course (CC - 3 & DSE - 1) will be of 4 credits each in addition to research projects for 6 Credits. The practical courses will be integral part of theory courses and no mention of practical courses separately.

Research projects are made compulsory during Sem – III and IV for all the students. A project (during Sem-III & IV) can be on theoretical Chemistry, experimental Chemistry, applied Chemistry, development Chemistry, computational Chemistry or industrial product development. A student earns 22 (twenty-two) credits per semester and total of 88 (Eighty Eight) credits in four semesters. The course structure is as follows:

Theory Courses:

SEM	Core Courses (CC)			Discipline Specific Elective (DSE) Course		RM
III	**Course - 1: Theoretical Organic Chemistry I (4) Course Code – CHE501**	**Course – 2: Methods in Organic Synthesis I (4) Course Code – CHE502**	**Course – 3: Advanced Organic Chemistry (6) Course Code – CHE503**	**Course – 4A: (4) Pharmaceutical and Forensic Science Course Code – CHE504A**	**Course – 4B: (4) Industrial Pharmacy Course Code – CHE504B**	**Course – 5: Research Projects (4) Course Code – CHE505**
IV	**Course - 1: Theoretical Organic Chemistry II (4)**	**Course – 2: Methods in Organic Synthesis II (4) Course Code –**	**Course – 3: Natural Products and Heterocyclic Chemistry (4)**	**Course – 4A: Intellectual Properties and Chemo-informatics (4)**	**Course – 4B: Quality Management Systems and Audit (4) Course Code –**	**Course – 5: Research Projects (6) Course Code –**

	Course Code – CHE551	**CHE552**	**Course Code – CHE553**	**Course Code – CHE554A**	**CHE554B**	**CHE555**

SEMESTER – III

M.Sc. in Chemistry Program for Semester-III consists of FOUR theory courses and practicals are integral parts of theory courses and research projects. The details are as follows:

Theory Courses (5): 20 hours per week (One lecture is of one-hour duration)

Course Code	Name of the Course	Lectures (Hrs.)	Practicals (Hrs.)	Total (Hrs)
CHE501	**Theoretical Organic Chemistry (4 Credits)**	45	30	75
CHE502	**Methods in Organic Synthesis I (4 Credits)**	45	30	75
CHE503	**Advanced Organic Chemistry (4 Credits)**	60	60	120
CHE504A/ CHE504B	**Industrial Pharmacy/ Regulatory affairs in PharmaceuticalIndustry (4 Credits)**	45	30	75
CHE505	**Research Projects (6 Credits)**	---	120	120
	TOTAL =	**195**	**270**	**465**

SEMESTER - IV

M.Sc. in Chemistry Program for Semester-IV consists of FOUR theory courses and practical are integral part of theory courses and research projects. The details are as follows:

Theory Courses (5): 20 hours per week (One lecture is of one-hour duration)

Course Code	Name of the Course	Lectures	Practicals	Total

		(Hrs.)	(Hrs.)	(Hrs)
CHE551	**Theoretical Organic Chemistry II (4 Credits)**	45	30	75
CHE552	**Methods in Organic Synthesis II (4 Credits)**	45	30	75
CHE553	**Natural Products and HeterocyclicChemistry (4 Credits)**	45	30	75
CHE554A/ CHE554B	**Intellectual Properties and Chemoinformatics / Quality Management Systems and Audit – II (4 Credits)**	45	30	75
CHE555	**Research Projects (6 Credits)**	---	180	180
	TOTAL =	**180**	**300**	**480**

The candidate shall be awarded the degree of ***Master of Science in Chemistry*** **(M. Sc. In Chemistry – Materials Science)** after completing

the course and meeting all the evaluation criteria.

2. Passing Standards:

- This course will have 40% Continuous Internal Evaluation (CIE) and 60% Semester End Examination (SEE) (written examination of 2.5 Hours duration for each theory course and practical examination of 4 Hours duration for each practical course). All external examinations will be held at the end of each semester and will be conducted by the college as per the existing norms of the University.
- Continuous Internal Evaluation (CIE) and 60% Semester End Examination (SEE) - shall have separate heads of passing. For Theory courses, continuous internal evaluation shall carry 40 marks and Semester-end examination shall carry 60 marks for each Theory Course.
- To pass, a student has to obtain minimum grade point E or above separately in CIE and the SEE examinations.
- The external examination for all Theory and Practical courses shall be conducted at the end of each Semester and the evaluation of min projects will be conducted at the end of I & II. The evaluation of Internship work will be conducted at the end of Sem-III and

evaluation of Project Dissertation will be conducted at the end of the fourth Semester.

- The candidates shall appear for external examination of 5 theory courses each carrying 60 marks of 2.5 hours duration and two practical courses in each of the semesters – I, II, III & IV, each carrying 100 marks at the end of each semester.
- The candidate shall prepare and submit for practical examination, a certified Journal based on the practical courses carried out under the guidance of a faculty member with minimum number of experiments as specified in the syllabus.
- The candidate shall submit an Internship report or Certificate before appearing for third semester end examination and Project Report / Dissertation for the Project Topic at the end of fourth semester as per the guidelines.

3. Standard point scale for grading:

Marks	**Grade Points**	**Grade**	**Performance**
80.00 and Above	10	O	Outstanding
70 to 79.99	9	A+	Excellent
60 to 69.99	8	A	Very Good
55 to 59.99	7	B+	Good
50 to 54.99	6	B	Above Average
45 to 49.99	5	C	Average
40 to 44.99	4	D	Pass
Less Than 40	1	F	Fail

4. Grade Point Average (GPA) calculation:

1. GPA is calculated at the end of each semester after grades have been processed and after any grades have been updated or changed. Individual assignments / quizzes / surprise tests / unit tests / tutorials / practicals / project / seminars etc. as prescribed by University are all based on the same criteria as given above. The teacher should convert his marking into the Quality-Points and Letter-Grade.
2. Performance of a student in a semester is indicated by a number called Semester Grade Point Average (SGPA). It is the weighted average

of the grade points

$$CGPA = \Sigma_{i=1} Cipi / \Sigma_{i=1} Ci$$

Ci = The number of credits earned in the i^{th} course of a semester.
pi = Grade point earned in the i^{th} course.
i = 1, 2, ….n represents number of courses for which the student is registered.

3. The Final remark grade will be decided on the basis of Cumulative Grade Point Average (CGPA) which is weighted average of the grade points obtained in all the semesters registered by the learner.

$$CGPA = \Sigma_{j=1} C_j p_j / \Sigma_{j=1} Cj$$

Cj = The number of credits earned in the jth course up to the semester for which the CGPA is calculated.
pj = Grade point earned in the jth course*
j = 1,2,…. n represents number of courses for which the student is registered up to the semester for which the CGPA is calculated.

National Education Policy 2020 with effect from the academic year 2023- 2024

M.Sc.-II Organic Chemistry Semester – III (22 Credits)

Sem I

Unit	Topics	Credits	L/Week
Core Course I – CHE501**: Theoretical Organic Chemistry I**			
Unit I	**Pericyclic reactions**	**3**	**1**
Unit II	**Stereochemistry-I**		**1**
Unit III	**Photochemistry**		**1**
Core Course II – CHE502**: Methods in Organic Synthesis I**			
Unit I	**Name Reactions with Mechanism and Application**		**1**

Unit II	**Enamines, Ylides and α-C-H Functionalization**	**3**	**1**
Unit III	**Metals / Non-metals in Organic Synthesis**		**1**
DSE Course I – CHE503 **: Advanced Organic Chemistry**			
Unit I	**Natural Products I and Green Chemistry**	**3**	**1**
Unit II	**Advanced Spectroscopic Techniques-I**		**1**
Unit III	**Advanced Spectroscopic Techniques-II**		**1**
CHE5**04 A: Industrial Pharmacy**			
Unit I	**General Guidelines in Pharmaceutical Industry**	**2**	**1**
Unit II	**Documentation in Pharmaceutical Industry**		**1**
CHE504 **B: Intellectual Property Rights and Cheminformatics**			
Unit I	**Introduction to Intellectual Property [15]**	**2**	1
UNIT II	**Chemoinformatics and its Applications**		1
Core Course Practical I – CHEP501**: Separation of a Ternary Mixture**			
	Separation of a solid ternary mixture using micro-scale technique	**1**	
Core Course Practical II – CHEP5**02: Derivative Preparation**			
	Identification of two components present in it.	**1**	
Course Practical III – CHE503 **A:** Single-Step **Preparation**			
	Derivative of Different types of compounds	**1**	
Course Practical IV - PGCHOPDSE304 B: Single-Step **Preparation**			

	Single step organic preparation (1.0 g scale) involving, techniques of purification. Single-step **organic preparation (1.0 g scale) involving, techniques of purification and green methods of synthesis**	**2**	

M.Sc.-II Organic Chemistry Semester – IV (22 Credits)

Unit	Topics	Credits	L/Week
Core Course I CHE551 **-: Theoretical Organic Chemistry II (4 Credits)**			
Unit I	Supramolecular Chemistry	3	**1**
Unit II	Stereochemistry-II		**1**
Unit III	Asymmetric Synthesis		**1**
Core Course II CHE552 - **Methods in Organic Synthesis II (4 Credits)**			
Unit I	Designing Organic Synthesis I	3	**1**
Unit II	Electro-organic Chemistry and Selected Methods of Organic Synthesis		**1**
Unit III	Transition and Rare Earth Metals in Organic Synthesis		**1**
Core **Course I –** CHE553 **: Natural Products and Heterocyclic Chemistry**			
Unit I	Natural Products III	3	**1**
Unit II	Heterocyclic Compounds I		**1**
Unit III	Heterocyclic Compounds-II		**1**

Elective CHE554 **A: Quality Management Systems and Audit**			
Unit I	Quality Management Systems and the ISO 9000 Series of Standards	2	**1**
Unit II	The Audit Process		**1**
Elective CHE554**B:Intellectual Property Rights and Cheminformatics** and its applications			
Unit I	Introduction to Intellectual Property	2	**1**
Unit III	Cheminformatics and their Applications		**1**
Core Course Practical I & **II –** CHE551 & CHE552**: Two Stage Preparation**			
	Two-Stage Organic Preparation	2	
Core Course Practical II & III **–** CHE552 & CHE553**: Two Stage Preparation**			
	Two-Stage Organic Preparation	2	
DSE Course Practical IV PGCHOPDSE404 B: Interpretation of Spectral Data			
	Interpretation of spectral data	**1**	

M.Sc II Sem III Organic Chemistry

Theory Courses

SEMESTER - III

Core Course I – CHE501: Theoretical Organic Chemistry I

Course Code: CHE501 (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CO-PO-PSO Mapping

Semester-III

CHE501: Theoretical Organic Chemistry I

After successful completion of each course in Chemistry a learner should be able to:

1. To explain various concepts in photochemistry pericyclic reactions and conformation of cyclohexane. (2)
2. To describe, classify and predict the reaction mechanism using reactive intermediates and from different pericyclic and photochemical reactions. (2, 5)
3. To apply concept of I-strain, Bredt's rule for cyclic compounds (3)

ICT Tools: Videos, PPT, Smart Board

Students Centric Methods: Experimental, Participative, Problem Solving

The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO-1	1	-	1	2	2	-	2	-	-	-	-	-	2	2	-
CO-2	2	1	2	-	-	-	-	-	-	-	-	-	-	2	-
CO-3	1	2	-	-	-	-	-	-	-	-	-	-	-	2	1

M.Sc II Sem III Organic Chemistry

Core Course I – CHE501: Theoretical Organic Chemistry I

Learning Objectives:

To learn the reactive intermediates and mechanism in organic synthesis.

1. To study pericyclic reactions and their types with mechanism.
2. To understand the stereochemistry of reactants, intermediates and products.
3. To study various types of photochemical reactions with mechanism

Unit I Pericyclic Reactions [15L]

1.1 Pericyclic reactions: Classification of pericyclic reactions; thermal and photochemical reactions. Three approaches: Evidence for the concertedness of bondmaking and breaking Symmetry-Allowed and Symmetry-Forbidden Reactions –

- The Woodward-Hoffmann Rules-Class by Class
- The generalized Woodward-Hoffmann Rule Explanations for Woodward-Hoffmann Rules
- The Aromatic Transition structures [Huckel and Mobius]
- Frontier Orbitals
- Correlation Diagrams, FMO and PMO approach
  Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene, 1,3,5 hexatriene and allyl system.

1.2 Cycloaddition reactions: Supra and antra facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes. Diels-Alder reactions, 1, 3-Dipolar cycloaddition and cheletropic reactions, ene reaction, retro-Diels-Alder reaction, regioselectivity, periselectivit, torquoselectivity, site selectivity and effect of substituents in Diels-Alder reactions. Other Cycloaddition Reactions- [4+6] Cycloadditions, Ketene Cycloaddition, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions. Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions.

1.3 Electrocyclic reactions: Conrotatory and disrotatary motions, 4nπ and [4n+2]π electron and allyl systems.

1.4 Sigmatropic rearrangements: H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxy- Copeand aza-Cope) and Claisen rearrangements. Formation of Vitamin D from 7-dehydrocholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A.

Unit II Stereochemistry-I [15L]

2.1 Classification of point groups based on symmetry elements with examples (nonmathematical treatment).

2.2 Conformational analysis of medium rings: Eight to ten membered rings and theirunusual properties, I-strain, transannular reactions.

2.3 Stereochemistry of fused ring and bridged ring compounds: decalins,hydrindanes, perhydroanthracenes, steroids, and Bredt's rule.

2.4 Anancomeric systems, Effect of conformation on reactivity of cyclohexane derivativesin the following reactions (including mechanism): electrophilic addition, elimination,molecular rearrangements, reduction of cyclohexanones (with LiAlH4, selectride andMPV reduction) and oxidation of cyclohexanols.

Unit III Photochemistry [15L]

3.1 Principles of photochemistry: quantum yield, electronic states and transitions, selection rules, modes of dissipation of energy (Jablonski diagram), electronic energy transfer: photosensitization and quenching process.

3.2 Photochemistry of carbonyl compounds: $\pi\rightarrow\pi^*$, $n\rightarrow\pi^*$ transitions, Norrish- I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of α, β-unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction.

3.3 Photochemistry of olefins: cis-trans isomerizations, dimerizations, hydrogen abstraction, addition and Di- π- methane rearrangement including aza-di- π - methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes.

3.4 Photochemistry of arenes: 1, 2- , 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings.

3.5 Singlet oxygen and photo-oxygenation reactions. Photochemically induced radical reactions. Chemiluminescence.

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28. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
29. Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri,3rd edition, New Age International Ltd.
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31. Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
32. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
33. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
34. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.

Core Course I – CHE502: Methods in organic synthesis I

Course Code: CHE502 (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CHE502: Methods in Organic Synthesis I
1. To explain various name reactions, radical reactions, enamines incorporated reactions, α-C-H functionalized reactions, etc. (2) 2. To predict the desired product using correct reaction mechanism. (5) 3. To construct a suitable organic synthesis using metal/ non-metallic reagents. (6) 4. To apply suitable mechanistic pathway for organic synthesis using ylides. (3)
ICT Tools: Videos, PPT, Smart Board
Students Centric Methods: Experimental, Participative, Problem Solving
The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	P O 8	P O 9	PO10	PO11	P O 1 2	P S O 1	PSO2	P S O 3
CO-2	2	-	-	2	2	-	-	-	-	-	-	-	2	2	-
CO-3	1	2		-	-	-	-	-	-	-	-	-	-	2	1
CO-5	2	1	2	-	-	-	-	-	-	-	-	-	-	2	-
CO-6	1	-	-	-	2	-	-	-	-	-	-	-	1	-	-

Core Course II – CHE502: Methods in Organic Synthesis I

Learning Objectives:

1. To learn various name reactions in organic synthesis.
2. To study organic free radical and their importance in organic synthesis.
3. To understand the applications of enamines, ylides and α C-H functionalization in organic synthesis. know the applications of organometallic compounds

Unit I Name Reactions with Mechanism and Application [15L]

1.1 Mukaiyama esterification, Mitsunobu reaction, Darzen's Glycidic Ester syntheis, Ritter reaction, Yamaguchi esterification, Peterson olefination.

1.2 Domino reactions: Characteristics; Nazerov cyclization

1.3 Multicomponent reactions: Strecker Synthesis, Ugi 4CC, Biginelli synthesis, Hantzsch synthesis, Pictet-Spengler synthesis

1.4 Click Reactions: Characteristics, Huisgen 1,3-Dipolar Cycloaddition.

Unit II Enamines, Ylides and α -C-H Functionalization [15]

2.1 Enamines: Generation and application in organic synthesis with mechanistic pathways, Stork enamine reaction. Reactivity, comparison between enamines and enolates. Synthetic reactions of enamines including asymmetric reactions of chiral enamines derived from chiral secondary amines.

2.2 Phosphorus, Sulfur and Nitrogen Ylides: Preparation and their synthetic applications along

with their stereochemical aspects. Wittig reaction, Horner-Wadsworth- Emmons Reaction, Barton-Kellogg olefination.

2.3 α-C-H functionalization: By nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Bamford-Stevens reaction, Julia olefination and its modification, Seyferth–Gilbert homologation, Steven's rearrangement.

Unit III Metals / Non-metals in Organic Synthesis [15]

3.1 Mercury in organic synthesis: Mechanism and regiochemistry of oxymercuration and demercuration of alkenes, mercuration of aromatics, transformation of aryl mercurials to aryl halides. Organomercurials as carbene transfer reagents.

3.2 Organoboron compounds: Mechanism and regiochemistry of hydroboration of alkenes and alkynes, asymmetric hydroboration using chiral boron reagents, 9-BBN hydroboration, oxazaborolidine (CBS catalyst) and functional group reduction by diborane.

3.3 Organosilicons: Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allyl silanes. β-silyl cations as intermediates. Iodotrimethylsilane in organic synthesis.

3.4 Silyl enol ethers: Application: As nucleophiles (Michael reaction, Mukaiyama aldol reaction), in ring contraction reactions.

3.5 Organotin compounds: Preparation of alkenyl and allyl tin compounds; application in C-C bond formation, in replacement of halogen by H at the same C atom.

3.6 Selenium in organic synthesis: Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno acetals as α-C-H activating groups.

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5. Moder Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
6. Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press (2002).
7. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3rd Edn., Nelson Thornes
8. Organic Chemistry, 7th Edn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson
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10. Advanced Organic Chemistry: Reactions & Mechanisms, 2nd Edn., B. Miller & R. Prasad, Pearson
11. Organic reactions and their mechanisms, 3rd revised edition, P.S. Kalsi, New Age International Publishers
12. Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley &

Sons, 2004
13. Name Reactions and Reagents in Organic Synthesis, 2nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
14. Name Reactions, Jie Jack Lie, 3rd Edn., Springer
15. Organic Electrochemistry, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Core Course I – CHE503: Advanced Organic Chemistry

Course Code: CHE502 (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CHE503: Advanced Organic Chemistry
1. To describe various components and concepts in PMR as well as CMR spectroscopic techniques. (2) 2. To deduce the structure of organic compounds using given spectral data. (3,5) 3. To explain the structural features and applications of different natural products. (2) 4. To elucidate the structure of various natural products. (4)
Students Centric Methods: Experimental, Participative, Problem Solving
The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	P O 8	P O 9	PO10	PO11	P O 1 2	P S O 1	P SO2	P S O 3
CO-2	1	-	2	2	-	-	-	-	-	-	2	-	-	2	-
CO-3	1	2		-	-	-	-	-	-	-	1	-	-	2	1
CO-4	2	1	2	-	-	-	-	-	-	-	1	-	-	2	-
CO-5	1	-	-	-	2	-	-	-	-	-	-	-	1	-	-

*In CO-PO Mapping Matrix: A correlation is established between COs and POs in the scale of 1 to 3, 1 being the slight (low), 2 being moderate (medium), 3 being substantial (high) and '-' indicate there is no correlation in respective CO and PO & PSO.

CHE Course III – CHE503: Advanced Organic Chemistry

Learning Objectives:

1. To learn the basic concepts involved in natural products.
2. To study the multi-step synthesis of various natural products.
3. To learn the advance spectroscopic technique for analysis of organic compound.
4. To understand advance instrumental techniques for compound interpretation and

identification.

Unit I Natural Products-I [15L]

1.1 Carbohydrates: Introduction to naturally occurring sugars: Deoxy sugars, Amino sugars, branched sugars. Structure elucidation of lactose and D- glucosamine (synthesis not expected).Structural features and applications of inositol, starch, cellulose, chitin and heparin.

1.2 Insect pheromones: General structural features and importance. Types of pheromones (aggregation, alarm, releaser, primer, territorial, trail, sex pheromones etc.), the advantage of pheromones over conventional pesticides. Synthesis of bombykol from acetylene, disparlure from 6-methylhept-1-ene, grandisol from 2-methyl-1, 3- butadiene.

1.3 Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, greencatalysts.

1.4 Green Cataysts: Nanocatalyst, Types of nanoctalysts, Advantages and Disadvantagesof nanocatalysts, Idea of Magnetically separable nanocatalysts.

Unit II Advanced Spectroscopic Techniques-I [15L]

2.1 Proton NMR spectroscopy: Recapitulation, chemical and magnetic equivalence of protons, first order, second order, Spin system notations (A2, AB, AX, AB2, AX2, AMX and A2B2-A2X2 spin systems with suitable examples). Long range coupling (Allylic coupling, 'W' coupling and Coupling in aromatic and heteroaromatic systems), Temperature effects, Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents.

2.2 13C –NMR spectroscopy: Recapitulation, equivalent and non-equivalent carbons (examples of aliphatic and aromatic compounds), 13C- chemical shifts, calculation of 13C- chemical shifts of aromatic carbons, heteronuclear coupling of carbon to 19F and 31P.

2.3 Spectral problems based on UV, IR, 1HNMR and 13CNMR and Mass spectroscopy.

Unit III Advanced Spectroscopic Techniques-II [15L]

3.1 Advanced NMR techniques: DEPT experiment, determining number of attached hydrogens (Methyl/methylene/methine and quaternary carbons), two dimensional spectroscopic techniques, COSY and HETCOR spectra, NOE, NOESY and ROESY techniques.

3.2 Spectral problems based on UV, IR, 1HNMR, 13CNMR (Including 2D technique) andMass spectroscopy

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1. Nelson, D. L, and Cox, M. M, (2008) Lehninger principles of Biochemistry 5th Edition, W. H. Freeman and Company, NY., USA.
2. Stryer, Lubert; Biochemistry; W. H. Freeman publishers.
3. Voet, D. and J. G. Voet (2004) Biochemistry, 3rd Edition, John Wiley & sons, Inc. USA.
4. Zubay, Goffrey L; Biochemistry; Wm C. Brown publishers.
5. V. Polshettiwar, R. Luque, A. Fihri, H. Zhu, M. Bouhrara and J-M Basset, Chem. Rev.2011, 111, 3036-3075

6. R. B. Nasir Baig and R. S.Varma, Chem. Comm., 2013, 49, 752-770;
7. M. B. Gawande, A. K. Rathi, P. S. Varma, Appl. Sci., 2013, 3, 656-674;
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10. D. Astruc, Nanomaterials and Catalysis, Wiley-VCH Verlag GmbH & Co. KGaA, 2008,1-48;
11. C. N. R. Rao, A. Muller and A. K. Cheetham, The chemistry of Nanomaterials, Wiley-VCH Verlag GmbH & Co. KGaA, 2005, 1-11
12. The organic chemistry of drug design and drug action, Richard B. Silverman, 2nd edition, Academic Press
13. Medicinal chemistry, D.Sriram and P. Yogeeswari, 2nd edition, Pearson
14. An introduction to drug design-S. S. Pandeya and J. R. Dimmock (New age international)
15. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R. Mahadik and K.G. Bothara, Nirali prakashan.
16. Medicinal chemistry (Vol. I and II)-Burger
17. Strategies for organic drug synthesis and design - D. Lednicer Wiley
18. Pharmacological basis of therapeutics-Goodman and Gilman's (McGraw Hill)
19. Enzyme catalysis in organic synthesis, 3rd edition. Edited by Karlheinz Drauz, Harold Groger, and Oliver May, Wiley-VCH Verlag GmbH & Co KgaA, 2012.
20. Biochemistry, Dr U Satyanarayan and Dr U Chakrapani, Books and Allied (P) Ltd.
21. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
22. The Organic Chemistry of Enzyme-Catalysed Reactions, Academic Press, By Richard B. Silverman
23. Enzymes: Practical Introduction to structure, mechanism and data analysis, By Robert A. Copeland, Wiley-VCH, Inc.
24. The Organic Chemistry of Biological Pathways By John McMurry, Tadhg Begley by Robert and company publishers
25. Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B. G. Torssell, Apotekarsocieteten – Swedish pharmaceutical press.
26. Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House.
27. Natural Products Volume- 2, By O. P. Agarwal.
28. Chemistry of Natural Products, F. F. Bentley and F. R. Dollish, 1974.
29. Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.Ito Majori and S. Nozoo, Academic Press, 1974.
30. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.
31. Green Chemistry: An Introductory Text, 2nd Edition, Published by Royal Society of Chemistry, Authored by Mike Lancater.
32. Organic synthesis in water. By Paul A. Grieco, Blackie.
33. Green chemistry, Theory and Practical, Paul T. Anastas and John C. Warner.
34. New trends in green chemistry By V. K. Ahulwalia and M. Kidwai, 2nd edition, Anamaya Publishers, New Delhi.
35. An introduction to green chemistry, V. Kumar, Vishal Publishing Co.
36. Organic synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

Core Course I – CHE504A: Industrial Pharmacy

Course Code: CHE504A (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CHE504 A: Industrial Pharmacy
1. To Understand core concepts related to pharmacy, including biomedical sciences, manufacturing practices, and behavioral aspects. 2. To Analyze pharmaceutical challenges, think critically, and make informed decisions in daily practice. 3. To Recognize the role of a pharmacist in society, uphold ethical standards, and contribute to health and well-being.
ICT Tools: Videos, PPT, Smart Board
Students Centric Methods: Experimental, Participative, Problem Solving
The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	P O 8	P O 9	PO10	PO11	P O 1 2	P S O 1	P S O 2	P SO3
CO-2	1	1	2	-	-	-	-	-	-	-	-	-	-	2	-
CO-3	1	2		-	-	-	-	-	-	-	-	-	-	1	1
CO-4	2	-	-	2	2	-	-	-	-	-	-	-	2	2	-

CHE504 A: Industrial Pharmacy

Unit I General Guidelines in Pharmaceutical Industry [15]

1.1 FDA Regulations in the pharmaceutical industry, Concept, need and the Schedule of Audit.

1.2 Concept of sampling in the pharmaceutical industry and M Sampling protocols.

1.3 Concept of ICH guidelines in the pharmaceutical industry, FDA and SUPAC Guidelinesin the pharmaceutical industry.

Unit II Documentation in Pharmaceutical Industry [15]

2.1 Audit and Documentations in relation to pharmaceutical industry.

2.2 Document filing and the documents BMR in the pharmaceutical industry, Other Documentation for Quality Assurance in the pharmaceutical industry.

2.3 Process Analytical Technology (PAT), Concept of Raw Material Q.C, Flow of raw materials in manufacturing Facility in industry.

REFERENCE

1. The Theory and Practice of industrial Pharmacy by Leon Lachman, Herbert A. Lieberman.
2. Remington's Science and Practice of Pharmacy by A. Gennaro.
3. Ansel's Pharmaceutical Dosage form and Drug delivery system by Loyd V. Allen, Jr. Nicholas, G. Popovich, Howard C. Ansel.
4. Generic Drug Product Development by Leon Shargel and Isadore Kanfer.
5. Dispensing for Pharmaceutical Students by SJ Carter.
6. Pharmaceutical Packaging Technology by UK Jain, DC Goupale S Nayak.

Core Course I – CHE504B: Regulatory Affairs in Pharmaceutical Chemistry

Course Code: CHE504B (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CHE504 B: Regulatory affairs in Pharmaceutical Industry
1. To define the various concepts in IPR, trade secrets, cheminformatics, etc. (1) 2. To apply the computer assisted drug design and development. (3) 3. To investigate the representation of molecules chemical reactions and searching chemical structures. (5) 4. To classify the different international agreements with respect to WTO and Paris convention. (2,5)
ICT Tools: Videos, PPT, Smart Board
Students Centric Methods: Experimental, Participative, Problem Solving
The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO-2	1	1	2	-	-	-	-	-	-	-	-	-	-	2	-
CO-3	1	2		-	-	-	-	-	-	-	-	-	-	1	1
CO-4	2	-	-	2	2	-	-	-	-	-	-	-	2	2	-
CO-6	1	-	-	2	2	-	-	-	-	-	-	-	1	-	-

CHE504 B : Regulatory Affairs in Pharmaceutical Chemistry

UNIT I Drug Regulatory Affairs [15]

1.1 A detailed study of Federal Food, Drugs and Cosmetics Act of USA, restricted to human drugs, cosmetics and biotechnological products, with special emphasis on: a. History

of drug regulation in USA. b. Organization and functions of FDA, including historical developments. c. General definitions. d. Adulterated & misbranded drugs/cosmetics/biotechnological products. e. OTC drugs, Orphan drugs, Orange Book and Fast Track Products. f. General penalties as applicable to drugs, cosmetics and biotechnological Products.

UNIT II A detailed study of Federal Food, Drugs and Cosmetics [15]

2.1 A detailed study of Federal Food, Drugs and Cosmetics Act of USA, restricted to human drugs, cosmetics and biotechnological products, with special emphasis on: a. General drug approval process. b. Investigational New Drug application (INDA). c. New Drug Application (NDA) and BLA. d. ANDA. e. SNDA, SUPAC and BACPAC. f. Post marketingsurveillance.

Core Course Practical I-CHEP501: Separation of Ternary Mixture

Learning Objectives:

1. To learn separation techniques of the ternary mixture.
2. To identify the organic compounds and to prepare their respective derivatives

Separation of a Solid Ternary Mixture using Micro-Scale Technique

1. Separation of solid components of a ternary mixture (water-insoluble/soluble including carbohydrates) based upon differences in the physical and the chemical properties of the components.

Core Course Practical II - PGCHOP302: Identification of two components

1. Identification of the two components (indicated by the examiner) using micro-scale technique.Purification of the three components, measurement of their mass, and determinationof their physical constants.
2. Calculation of percentage yields of the individual components. (Identification of the components is not expected).

Core Course Practical III – CHE503: Derivative Preparation

Preparation of derivatives (any one of the separated compounds). (Minimum 8 experiments)

Course Practical IV-CHEP504 A: Single Step Preparation

Single-step organic preparation (1.0 g scale) involves purification techniques and green synthesis methods.

REFERENCE

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

Course - 5: Research Projects (CC)
Course Code: CHE505 (120 Hrs, 4 credits)

Course Outcomes (COs): After completion of this course, students should be able to …

CO1 : Research Skills Development: to formulate research questions, conduct literature reviews, design appropriate methodologies, collect and analyze data, and draw conclusions based on evidence.

CO2 : Critical Thinking: to develop critical thinking skills by questioning assumptions, analyzing evidence, and synthesizing information to form their own conclusions.

CO3 : Communication Skills: to develop effective communication skills, including the ability to articulate ideas clearly, structure arguments logically, and present information in a compelling manner.

CO4 : Problem-Solving Abilities: to learn to identify problems, develop strategies for addressing them, and adapt their approach as needed, involve encountering obstacles and challenges that require creative problem-solving skills.

SEMESTER - IV

Core Course I – CHE551: Theoretical Organic Chemistry II

Course Code: CHE551 (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CO-PO-PSO Mapping

Semester-IV

CHE551: Theoretical Organic Chemistry II

After successful completion of each course in Chemistry a learner should be able to:
1. To interpret Hammet and Taft equation for understanding reaction mechanism.
(4) 2. To study and apply various reagents for asymmetric synthesis. (2,3)
3. To deduce stereochemical outcomes by using axial halo ketone rule, Cotton effect, ORD & CD, etc.
(4) 4. To predict the synthetic products by using various supramolecules as a starting material.

ICT Tools: Videos, PPT, Smart Board

Students Centric Methods: Experimental, Participative, Problem Solving

The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	P S O 3
CO-2	1	-	1	2	2	-	2	-	-	-	-	-	2	2	-
CO-3	2	1	2	-	-	-	-	-	-	-	-	-	-	2	-
CO-4	1	2	-	-	-	-	-	-	-	-	-	-	-	2	1
CO-5	1	-	-	-	2	-	-	-	-	-	-	-	1	-	-

M.Sc II Sem IV Organic Chemistry

Core Course I – CHE551: Theoretical Organic Chemistry II

Unit I Theoretical Organic Chemistry and Supramolecular Chemistry [15]

1.1 Structural effects and reactivity: Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of σ- values, reaction constants ρ, Yukawa-Tsuno equation.

1.2 Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins, and enzymes.

1.3 Synthetic molecular receptors: receptors with a molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.

1.4 Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands andcalixarenes.

Unit II Stereochemistry- II [15]

2.1 Racemisation and resolution of racemates including conglomerates: Mechanism of racemisation, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds.

2.2 Determination of enantiomer and diastereomer composition: enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents(LSR).

2.3 Correlative method for configurational assignment: chemical, optical rotation and NMR spectroscopy.

2.4 Molecular dissymmetry and chiroptical properties: Linearly and circularly polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial α– haloketone rule with applications.

Unit III Asymmetric Synthesis [15]

3.1 Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methodsof asymmetric induction – substrate, reagent and catalyst controlled reactions.

3.2 Synthesis of L-DOPA [Knowles's Mosanto process]. Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharpless enantioselective epoxidation, hydroxylation, aminohydroxylation, Diels-Alderreaction, reduction of prochiral carbonyl compounds and olefins.

3.3 Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification.Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations.

REFERENCE

1. March's Advanced Organic Chemistry, Jerry March, sixth edition, 2007, John Wiley and sons.
2. A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi.
3. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).
4. Mechanism and theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.
5. Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.
6. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan Publishers, India.
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Ltd., London 1969.
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11. Organic Chemistry, Seventh Edition, R.T. Morrison, R. N. Boyd & S. K. Bhattacharjee, Pearson.Advanced Organic Chemistry: Reactions & Mechanisms, second edition, B. Miller and R. Prasad, Pearson.
12. Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
13. Organic Chemistry: Structure and Function, P. Volhardt and N. Schore, 5th Edition, 2012
14. Organic Chemistry, W. G. Solomons, C. B. Fryhle, , 9th Edition, Wiley India Pvt. Ltd.,2009.
15. Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.
16. Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
17. Pericyclic reactions, Ian Fleming, Oxford university press, 1999.
18. Pericyclic reactions-A mechanistic approach, S. M. Mukherji, Macmillan Co. of India 1979.
19. Organic chemistry, 8th edition, John McMurry
20. Modern methods of Organic Synthesis, 4th Edition W. Carruthers and Iain Coldham, Cambridge University Press 2004
21. Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books,2006
22. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
23. Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd.
24. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit
25. Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
26. Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
27. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
28. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
29. Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
30. Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.
31. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley- Eastern
32. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.
33. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
34. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
35. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
36. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.

Core Course II – CHE552: Methods in Organic Synthesis II

Course Code: CHE552 (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CHE552: Methods in Organic Synthesis II

1. To construct, design and create different target molecules by using proper precursor. (3,4,6) 2. To understand basic concepts in retrosynthetic analysis and electro-organic chemistry. (2) 3. To explain and predict the correct product in various coupling reactions. (2,5)
4. To deduce the organic synthesis by using transition and rare earth metals. (4)

ICT Tools: Videos, PPT, Smart Board

Students Centric Methods: Experimental, Participative, Problem Solving

The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO-2	2	-	-	2	2	-	-	-	-	-	-	-	2	2	-
CO-3	1	2		-	-	-	-	-	-	-	-	-	-	2	1
CO-5	2	1	2	-	-	-	-	-	-	-	-	-	-	2	-
CO-6	1	-	-	-	2	-	-	-	-	-	-	-	1	-	-

Core Course II – CHE552: Methods in Organic Synthesis II

Learning Objectives:

1. To learn the synthetic planning and designing in various organic synthesis.
2. To understand the methodology, basics, and applications of electro-organicchemistry.
3. To study applications of organometallics (transition and rare earth elements) in organic synthesis.

Unit I Designing Organic Synthesis-I [15L]

1.1 Protecting groups in Organic Synthesis: Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.

1.2 Concept of umpolung (Reversal of polarity): Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.

1.3 Introduction to Retrosynthetic analysis and synthetic planning: Linear and convergent synthesis; Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions (FGI), functional group addition (FGA), functional group removal (FGR) importance of order of events in organic synthesis, one and two group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds), selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity.

Unit II Electro-Organic Chemistry and Selected Methods of Organic Synthesis [15]

2.1 Electro-organic chemistry:

3.1.1 Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes.

3.1.2 Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins, arenes, electro-dimerization.

3.1.3 Anodic oxidation: Oxidation of alkylbenzene, Kolbe reaction, Non-Kolbe oxidation, Shono oxidation.

2.2 Selected Methods of Organic synthesis

Applications of the following in organic synthesis:

2.2.1 Organocatalysts: Proline, Imidazolidinone.

2.2.2 Pd catalysed cycloaddition reactions: Stille reaction, Saeguse-Ito oxidationto enones, Negishi coupling.

2.2.3 Use of Sc(OTf), and Yb(OTf) as water tolerant Lewis acid catalyst in aldol condensation, Michael reaction, Diels-Alder reaction, Friedel – Crafts reaction.

Unit III Transition and Rare Earth Metals in Organic Synthesis [15L]

3.1 Introduction to basic concepts: 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion.

3.2 Palladium in organic synthesis: π-bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerisation, cross-coupling of organometallics and halides. Representative examples: Heck reaction, Suzuki-Miayura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S or P atoms.

3.3 Application of Ni, Co, Fe, Rh, and Cr carbonyls in organic synthesis.

3.4 Application of samarium iodide including reduction of organic halides, aldehydes andketones, α-functionalized carbonyl and nitro compounds.

3.5 Application of Ce (IV) in the synthesis of heterocyclic quinoxaline derivatives and its roleas a de-protecting agent.

REFERENCE

1. Advanced Organic Chemistry, Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag
2. Modern Methods of Organic Synthesis, 4th Edition, W. Carruthers and Iain Coldham,

Cambridge University Press, 2004.
3. Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis, S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam.
4. Organic Chemistry, Clayden Greeves Warren and Wothers, Oxford Press (2001).
5. Moder Organic Synthesis: An Introduction, G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).Advanced Organic Chemistry: Reaction Mechanism, R. Bruckner, Academic Press(2002).
6. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3rd Edn., Nelson Thornes
7. Organic Chemistry, 7th Edn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson
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9. Advanced Organic Chemistry: Reactions & Mechanisms, 2nd Edn., B. Miller & R. Prasad, Pearson
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12. Name Reactions and Reagents in Organic Synthesis, 2nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
13. Name Reactions, Jie Jack Lie, 3rd Edn., Springer
14. Organic Electrochemistry, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Core Course III – CHE553: Natural Products and Heterocyclic Chemistry

Course Code: CHE553 (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CHE553: Natural Products and Heterocyclic Chemistry
. To understand the various parameters Viz. QSAR, Hansch analysis, multiple regression analysis, etc for drug design and development. (2) 2. To classify various drugs as per their therapeutic actions. (4) . To distinguish and classify the heterocyclic**PGCHODSE404** compounds on the basis of heteroatom present in the ring system. (4) 4. To predict the desired product with correct reaction mechanism in heterocyclic as well as drug chemistry.
Students Centric Methods: Experimental, Participative, Problem Solving
The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO-2	1	-	2	2	-	-	-	-	-	-	2	-	-	2	-

CO-3	1	2		-	-	-	-	-	-	-	1	-	-	2	1
CO-4	2	1	2	-	-	-	-	-	-	-	1	-	-	2	-
CO-5	1	-	-	-	2	-	-	-	-	-	-	-	1	-	-

Core Course III CHE553 : Natural Products and Heterocyclic Chemistry

Learning Objectives:

1. To learn the importance of steroids, vitamins and terpenoids in natural products.
2. To study the heterocyclic chemistry (3-6 membered rings) and their applications in organic synthesis.

Unit I Natural Products-III [15L]

1.1 Steroids: General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following: corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bile acid. Synthesis of 16-DPA from cholesterol and plant sapogenin.

1.2 Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone.

1.3 Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone.

1.4 Vitamins: Classification, sources and biological importance of vitamin B1, B2, B6, folic acid, B12, C, D1, E (α-tocopherol), K1, K2, H (β- biotin).

Synthesis of the following:

- Vitamin A from β-ionone and bromoester moiety.
- Vitamin B1 including synthesis of pyrimidine and thiazole moieties
- Vitamin B2 from 3, 4-dimethylaniline and D(-)ribose
- Vitamin B6 from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethyl esterof N-formyl-DL-alanine (Harris synthesis)
- Vitamin E (α-tocopherol) from trimethylquinol and phytyl bromide
- Vitamin K1 from 2-methyl-1, 4-naphthaquinone and phytol.

Unit II Heterocyclic Compounds-II [15L]

3.1 Heterocyclic compounds: Introduction, classification, Nomenclature of heterocyclic compounds of monocyclic (3-6 membered) (Common, systematic (Hantzsch- Widman) and replacement nomenclature)

3.2 Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazines, pyrimidine, pyrazines and oxazines.

Unit III Heterocyclic Compounds-II [15L]

4.1 Nomenclature of heterocyclic compounds of bicyclic/tricyclic(5-6 Membered) fused heterocycles (up to three hetero atoms). (Common, systematic (Hantzsch-Widman) and replacement nomenclature), Nucleophilic ringopening reactions of oxiranes, aziridines, oxetanes and azetidines.

4.2 Structure, reactivity, synthesis and reactions of coumarins, quinoxalines, cinnolines, indole, benzimidazoles, benzoxazoles, benzothiazoles, Purines and acridines.

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3. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011.
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DSE A – CHE554A: Natural Products and Heterocyclic Chemistry

Course Code: CHE554A (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CHE554A Quality Management Systems And Audit

The CO-PO Mapping Matrix

1. To understand the Quality management systems and the iso 9000 series of standards registration, certification and auditor competence
2. To evaluate the audit process
3. To apply Conducting the on-site audit

Students Centric Methods: Experimental, Participative, Problem Solving

The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO 7	PO8	PO9	PO10	PO11	PO12	PSO 1	PSO2	PSO 3	PSO4

CO-1	1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
CO-2	-	-	1	-	-	-	2	-	-	-	-	-	-	-	-	-
CO-3	-	-	-	-	1	-	-	-	-	-	-	-	-	-	-	-
CO-4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Elective– CHE554 A: Quality Management and Audit

UNIT I Quality Management Systems and the ISO 9000 Series of Standards [15]

1.1 The need for and benefits of a QMS • The ISO 9000 series of standards • ISO 9001:2015 fundamentals and vocabulary • Compatibility with other Standards • Legal compliance – ISO Standards • The process approach • The seven quality management principles

1.2 Process-Based Quality Management Systems
The application of PDCA Cycle, Quality system documented information, Electronic data systems, Control of documents and records, Monitoring and measurement, Infrastructure, Work environment, Product realization, Monitoring and measurement, continual improvement

UNIT III Audit Process [15]

2.1 Certification process, Planning the audit, Audit roles and responsibilities, Goodpractice at meetings

2.2 Preparing for the on-site Audit (Audit Stage 1)

2.3 Initial contact with the auditee, stage 1 audit, document review, the audit plan, workdocuments. Developing a Checklist: The audit checklist, process review, "Turtle Diagram"

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4. ISO 22000:2018. Food safety management systems — Requirements for any organization in the food chain.
5. ISO 14001:2015. Environmental management systems — Requirements withguidance for use.
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DSE B – CHE554B: Natural Products and Heterocyclic Chemistry

Course Code: CHE554B (45 Lectures of Theory and 30 hours of Practical, 4 credits)

CHE554B Intellectual Property Rights and Cheminformatics

The CO-PO Mapping Matrix

1 To understand the Introduction to Intellectual Property
2. To understand the trade Secrets of Cheminformatics
3.To illustrate the applications of Cheminformatics

Students Centric Methods: Experimental, Participative, Problem Solving

The CO-PO Mapping Matrix

CO\ PO	PO1	PO2	PO3	PO4	PO5	PO6	PO 7	PO8	PO9	PO10	PO11	PO12	PSO 1	PSO2	PSO 3	PSO4
CO-1	1	-	-	-	-	-	-	-	-	-	-	-	-	1	-	-
CO-2	-	-	1	-	-	-	-	-	2	-	-	-	-	-	-	-
CO-3	1	-	-	-	-	-	1	-	-	-	-	-	-	-	-	-
CO-4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

DSE – CHE554 B: Intellectual Property Rights and Cheminformatics and its applications

Unit I Introduction to Intellectual Property [15]

1.1 Introduction to Intellectual Property:
Historical Perspective, Different types of IP, Importance of protecting IP.

1.2 Patents:
Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.

1.3 Industrial Designs:
Definition, how to obtain, features, International design registration.

1.4 Copyrights:
Introduction, how to obtain, Differences from Patents.

1.5 Trade Marks
Introduction, how to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

1.6 Geographical Indications
Definition, rules for registration, prevention of illegal exploitation, importance to India.

1.7 Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

Unit II Cheminformatics and its Applications [15]

2.1 Introduction to Cheminformatics: History and evolution of cheminformatics, Use of Cheminformatics, prospects of cheminformatics, Molecular modeling and structure elucidation.

2.2 Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

2.3 Searching Chemical Structures:Full structure search, sub-structure search, basic ideas, similarity search, three-dimensional search methods, basics of computation of physical and chemical data and structure descriptors, and data visualization.

2.4 Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure–Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer-assisted Synthesis Design, Introduction to drug design, target identification and validation, lead finding and optimization, analysis of HTS data, virtual screening, design of combinatorial libraries, ligand-based and structure-based drug design, application of cheminformatics in drug design.

REFERENCE

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Course - 5: Research Projects (CC)
Course Code: CHE555 (180 Hrs, 6 credits)

Core Course Practical I – CHE551 & CHE552: Two Stage Preparation

Learning Objectives:

1. To learn the solubility and miscibility criteria for identification of unknown organic compounds.

Core Course Practical II – CHE552 & CHE553: Two Stage Preparation

Identification of any Unknown Organic Compound with Preparation, Purification and Physical Constant of Derivative. (Minimum 8 Organic Compounds) (Minimum 8 Experiments) (Double Stage Preparation)

DSE Course Practical III – : CHE554A Analysis of Spectral Data

Learning Objectives:

1. To learn the interpretation of the organic compounds by various spectroscopic techniques (UV, IR, PMR, CMR and Mass spectra).

INTERPRETATION OF SPECTRAL DATA OF ORGANIC COMPOUNDS (UV, IR, PMR, CMR AND MASS SPECTRA).

Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and Mass spectra). A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information should be reported within first half an hour of the examination without referring to any book/reference material. The complete structure of the compound may then be elucidated by referring reference material etc. (Minimum 8 spectral analysis)

DSE Course Practical IV – CHE554B Interpretation of SpectralData

INTERPRETATION OF SPECTRAL DATA OF ORGANIC COMPOUNDS (UV, IR, PMR, CMRAND MASS SPECTRA).

Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and Mass spectra). A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information should be reported within first half an hour of the examination without referring to any book/reference material. The complete

structure of the compound may then be elucidated by referring reference materialetc. (Minimum 8 spectral analysis)

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