MANONMANIAM SUNDARANAR UNIVERSITY
TIRUNELVELI - 12
PG - COURSES – AFFILIATED COLLEGES

M. Sc
CHEMISTRY

(Choice Based Credit System)

SYLLABUS

FROM THE ACADEMIC YEAR
2023-2024

MANONMANIAM SUNDARANAR UNIVERSITY TIRUNELVELI
PG - COURSES – AFFILIATED COLLEGES
M.Sc. CHEMISTRY
(Choice Based Credit System)
(For those who joined from 2023- 2024 onwards)

1. PREAMBLE

Taxonomy forms three learning domains: Cognitive (knowledge), affective (attitude) and psychomotor (skill). This classification enables to estimate the learning capabilities of students. Briefly, it is aimed to restructure the curriculum as student-oriented, skill-based, and institution-industry interaction curriculum with the various courses under "Outcome Based Education with Problem Based Courses, Project Based Courses, and Industry Aligned Programmes" having revised Bloom's Taxonomy for evaluating students' skills.

Cognitive Domain

(Lower levels: K1: Remembering; K2: Understanding; K3: Applying; Higher levels: K4: Analyzing; K5: Evaluating; K6: Creating)

Affective Domain

Psychomotor Domain.

All the changes in life in one-way or other involve chemistry. Chemistry is central to the current revolutions in science. No educated person today can understand the modern world without a basic knowledge of chemistry. The existence of a large number of chemical factories, mines and related industries necessitates chemistry education. An advanced course in chemistry will be a fascinating experience because it helps us understanding our surroundings. Hence, the Programme M.Sc. (Chemistry) is offered to meet current needs of aspiring youths and also create awareness about the in-depth scientific aspects to the society.

2. FRAMEWORK FOR POSTGRADUATE EDUCATION

MANONMANIAM SUNDARANAR UNIVERSITY, TIRUNELVELI - 12 PG - COURSES – AFFILIATED COLLEGES FRAMEWORK FOR POSTGRADUATE EDUCATION	
Programme	**M. Sc Chemistry**
Programme Code	
Duration	**PG – 2 YEARS**
Programme Outcomes (POs)	**PO1: Problem Solving Skill** Apply knowledge of Management theories and Human Resource practices to solve business problems through research in Global context. **PO2: Decision Making Skill** Foster analytical and critical thinking abilities for data-based decision-making. **PO3: Ethical Value** Ability to incorporate quality, ethical and legal value-based perspectives to all organizational activities. **PO4: Communication Skill** Ability to develop communication, managerial and interpersonal skills. **PO5: Individual and Team Leadership Skill** Capability to lead themselves and the team to achieve organizational goals. **PO6: Employability Skill** Inculcate contemporary business practices to enhance employability skills in the competitive environment. **PO7: Entrepreneurial Skill** Equip with skills and competencies to become an entrepreneur. **PO8: Contribution to Society** Succeed in career endeavors and contribute significantly to society. **PO9: Multicultural competence** Possess knowledge of the values and beliefs of multiple cultures and a global perspective. **PO10: Moral and ethical awareness/reasoning** Ability to embrace moral/ethical values in conducting one's life.

Programme Specific Outcomes (PSOs)	**PSO1 – Placement** Prepare the students who will demonstrate respectful engagement with others' ideas, behaviors, beliefs and apply diverse frames of reference to decisions and actions. **PSO2 – Entrepreneur** Create effective entrepreneurs by enhancing their critical thinking, problem solving, decision making and leadership skill that will facilitate startups and high potential organizations. **PSO3 – Research and Development** Design and implement HR systems and practices grounded in research that comply with employment laws, leading the organization towards growth and development. **PSO4 – Contribution to Business World** Produce employable, ethical and innovative professionals to sustain in the dynamic business world. **PSO5 – Contribution to the Society** Contribute to the development of the society by collaborating with stakeholders for mutual benefit.

3. Choice Based Credit System (CBCS), Learning Outcomes Based Curriculum Framework (LOCF) Guideline Based Credits and Hours Distribution System

First Year – Semester – I

Part	List of Courses	Credits	No. of Hours
	Core – I	4	5 (4L + 1T)
	Core – II	4	5 (4L + 1T)
	Core – III	3	5 (4P + 1T)
	Core - IV	3	5 (4P + 1T)
	Elective - I	3	5 (4L + 1T)
	Elective – II	3	5 (4L + 1T)
		20	**30**

Semester – II

Part	List of Courses	Credits	No. of Hours
	Core – V	4	5(4L + 1T)
	Core – VI	4	5(4L + 1T)
	Core – VII	3	4(3P + 1T)
	Core - VIII	3	4(3P + 1T)
	Elective - III	3	4(3L + 1T)
	Elective – IV	3	4(3L + 1T)
	Skill Enhancement Course - I	2	4
		22	**30**

Second Year – Semester – III

Part	List of Courses	Credits	No. of Hours
	Core – IX	5	6(5L + 1T)
	Core – X	5	6(5L + 1T)
	Core – XI	4	5(4P + 1T)
	Core (Industry Module) – XII	5	5(4P + 1T)
	Elective – V	3	4(3L + 1T)
	Skill Enhancement Course - II	2	4
	Internship / Industrial Activity [Credits]	2	-
		26	**30**

Semester-IV

Part	List of Courses	Credits	No. of Hours
	Core – XIII	5	6(5L + 1T)
	Core – XIV	5	6(5L + 1T)
	Project with VIVA VOCE	7	10
	Elective – VI (Industry Entrepreneurship)	3	4
	Skill Enhancement Course – III / Professional Competency Skill	2	4
	Extension Activity	1	-
		23	**30**

Total 91 Credits for PG Courses

4. COMPONENT WISE CREDIT DISTRIBUTION

Credits		Sem I	Sem II	Sem III	Sem IV	Total
Part A		**20**	**20**	**22**	**20**	**82**
Part B	**(i) Discipline – Centric / Generic Skill**		**2**	**2**	**2**	**6**
	(ii) Summer Internship / Industrial Training			**2**		**2**
Part C					**1**	**1**
	Total	**20**	**22**	**26**	**23**	**91**

Part A component and Part B (i) will be taken into account for CGPA calculation for the postgraduate programme and the other components Part B and Part C have to be completed during the duration of the programme as per the norms, to be eligible for obtaining the PG degree.

5. LEARNING AND TEACHING ACTIVITIES

5.1 Topic wise Delivery method

Hour Count	Topic	Unit	Mode of Delivery

5.2. Work Load

The information below is provided as a guide to assist students in engaging appropriately with the course requirements.

Activity	Quantity	Workload periods
Lectures	60	60
Tutorials	15	15
Assignments	5	5
Cycle Test or similar	2	4
Model Test or similar	1	3
University Exam	1	3
	Total	90 periods

6. TUTORIAL ACTIVITIES

Tutorial Count	Topic

7. LABORATORY ACTIVITIES

8. FIELD STUDY ACTIVITIES

9. ASSESSMENT ACTIVITIES

9.1. Assessment Principles

Assessment for this course is based on the following principles

1. Assessment must encourage and reinforce learning.
2. Assessment must measure achievement of the stated learning objectives.
3. Assessment must enable robust and fair judgments about student performance.
4. Assessment practice must be fair and equitable to students and give them the opportunity to demonstrate what they learned.
5. Assessment must maintain academic standards.

9.2. Assessment Details

Assessment Item	Distributed Due Date	Weightage	Cumulative Weightage
Assignment 1	3rd week	2%	2%
Assignment 2	6th Week	2%	4%
Cycle Test – I	7th Week	6%	10%
Assignment 3	8th Week	2%	12%
Assignment 4	11th Week	2%	14%
Cycle Test – II	12th Week	6%	20%
Assignment 5	14th Week	2%	22%
Model Exam	15th Week	13%	35%
Attendance	All weeks as per the Academic Calendar	5%	40%
University Exam	17th Week	60%	100%

10. TEACHING METHODOLOGIES

1. Traditional Teaching methods like Chalk and Board, Virtual Class room, LCD projector, Smart Class, Video Conference, Guest Lectures.
2. Asking students to formulate a problem from a topic covered in a week's time Assignment, Class Test, Slip test.
3. Asking students to use state-of-the-art technologies/software to solve problems. Applications: Use of chemdraw, chempaint software
4. Introducing students to applications before teaching the theory.
5. Training students to engage in self-study without relying on faculty (for example – library and internet search, manual and handbook usage, etc.)

   5.1 Library, Net Surfing, Manuals, NPTEL Course Materials published in the website

   5.2 Other university websites.

11. FACULTY COURSE FILE STRUCTURE

CONTENTS

a) Academic Schedule

b) Students Name List

c) Time Table

d) Syllabus

e) Lesson Plan

f) Staff Workload

g) Course Design (content, Course Outcomes (COs), Delivery method, mapping of COs with Programme Outcomes (POs), Assessment Pattern in terms of Revised Bloom's Taxonomy)

h) Sample CO Assessment Tools

i) Faculty Course Assessment Report (FCAR)

j) Course Evaluation Sheet

k) Teaching Materials (PPT, OHP etc.)

l) Lecture Notes

m) Home Assignment Questions

n) Tutorial Sheets

o) Remedial Class Record, if any

p) Projects related to the Course

q) Laboratory Experiments related to the Courses

r) Internal Question Paper

s) External Question Paper

t) Sample Home Assignment Answer Sheets

u) Three best, three middle level and three average Answersheets

v) Result Analysis (CO wise and whole class)

w) Question Bank for Higher studies Preparation (GATE/Placement)

x) List of mentees and their academic achievements

12. COURSE STRUCTURE

M. Sc. Chemistry

First Year - Semester - I

	Courses	**Credit**	**Hours per Week (L/T/P)**
Part A	Core Courses 4 (CC1, CC2, CC3, CC4)	14	20
	Elective Courses 2(Generic / Discipline Specific) EC1, EC2	6	10
		20	**30**

Semester-II

	Courses	**Credit**	**Hours per Week (L/T/P)**
Part A	Core Courses 4 (CC5, CC6, CC7, CC8)	14	18
	Elective Courses 2 (Generic / Discipline Specific) EC3, EC4	6	8
Part B	Skill Enhancement Course - SEC 1(One from Group G)	2	4
		22	**30**

Second Year – Semester - III

	Courses	**Credit**	**Hours per Week (L/T/P)**
Part A	Core Courses 4 (CC9, CC10, CC11, CC12)	19	22
	Elective Course 1 (Generic / Discipline Specific) EC5	3	4
Part B	Skill Enhancement Course - SEC 2 (One from Group G)	2	4
	Internship / Industrial Activity (Carried out in Summer Vacation at the end of I year – 30 hours)	2	
		26	**30**

Semester - IV

Part	**Courses**	**Credit**	**Hours per Week(L/T/P)**
Part A	Core Courses 2 (CC13, CC14)	10	12
	Project with Viva voce	7	10
	Elective Course 1 (Industry / Entrepreneurship) EC6	3	4

Part B	Professional Competency Skill Enhancement CourseTraining for Competitive Examinations • Chemistry for NET / UGC - CSIR/ SET / TRB Competitive Examinations (2 hours) • General Studies for UPSC / TNPSC / Other Competitive Examinations (2 hours)	2	4
Part C	Extension Activity (Can be carried out from Sem II to Sem IV)	1	
		23	**30**

13. Credit Distribution for PG Programme in Chemistry
M. Sc Chemistry

Illustration - I

	First Year Semester-I	**Credit**	**Hours per week (L/T/P)**
Part A	CC1 – Organic Reaction Mechanism-I	4	5(4L + 1T)
	CC2 – Structure and Bonding in Inorganic Compounds	4	5(4L + 1T)
	CC3 – Organic Chemistry Practical - I	3	5(4P + 1T)
	CC4 – Physical Chemistry Practical	3	5(4P+ 1T)
	Elective I – EC1 (One from Group A) Pharmaceutical Chemistry/Nanomaterials and Nanotechnology	3	5(4L + 1T)
	Elective II – EC2 (One from Group B) Electrochemistry/Molecular Spectroscopy	3	5(4L + 1T)
	Total	**20**	**30**

	Semester-II	**Credit**	**Hours per week(L/T/P)**
Part A	CC5 – Organic reaction mechanism-II	4	5(4L + 1T)
	CC6– Physical Chemistry-I	4	5(4L + 1T)
	CC7 – Organic Chemistry Practical - II	3	4(3P + 1T)
	CC8 – Inorganic Chemistry Practical - I	3	4(3P + 1T)
	Elective III–EC3 (One from Group C) Medicinal Chemistry/Green Chemistry	3	4(3L + 1T)
	Elective-IV-EC4 (One from Group D) Bio Inorganic Chemistry/Material Science	3	4(3L + 1T)
Part B	Skill Enhancement Course -SEC 1 (One from Group G) Computational Chemistry	2	4
	Total	**22**	**30**

14. CONSOLIDATED TABLE FOR CREDITS DISTRIBUTION

<table>
<tr><td rowspan="4">PART A</td><td>Category of Courses</td><td>Numberof Courses</td><td>Number of Credits in each Category of Courses</td><td>Total Credits</td><td>Total Credits for the Programme</td></tr>
<tr><td>Core</td><td>14</td><td>57</td><td rowspan="3">82</td><td rowspan="4">88 (CGPA)</td></tr>
<tr><td>Project with viva voce</td><td>1</td><td>7</td></tr>
<tr><td>Elective (Generic and Discipline Centric)</td><td>6</td><td>18</td></tr>
<tr><td>PART B (i)</td><td>Skill Enhancement (Term paper and Seminar & Generic / Discipline - Centric Skill Courses) (Internal Assessment Only)</td><td>3</td><td>6</td><td>6</td></tr>
<tr><td>PART B(ii)</td><td>Summer Internship</td><td>1</td><td>2</td><td>2</td><td rowspan="2">03 (Non CGPA)</td></tr>
<tr><td>PART C</td><td>Extension Activity</td><td>1</td><td>1</td><td>1</td></tr>
<tr><td colspan="4"></td><td></td><td>91</td></tr>
</table>

15. TEMPLATE FOR SEMESTER EXAMINATION

Code	Category	Title of the Paper	Marks (Max 100)		Duration for UE	Credits
			CIA	UE		
Semester –I						
Part A	Core I		25	75	3 Hrs	4
	Core II		25	75	3 Hrs	4
	Core III		25	75	3 Hrs	3
	Core IV		25	75	3 Hrs	3
	Elective I	Elective-I (Choose one from Group-A)	25	75	3 Hrs	3
	Elective II	Elective-II (Choose one from Group-B)	25	75	3 Hrs	3
Semester-II						
Part A	Core V		25	75	3 Hrs	4
	Core VI		25	75	3 Hrs	4
	Core VII		25	75	3 Hrs	3
	Core VIII		25	75	3 Hrs	3
	Elective III	Elective-III (Choose one from Group-C)	25	75	3 Hrs	3
	Elective IV	Elective-IV (Choose one from Group-D)	25	75	3 Hrs	3
Part B	Skill Enhancement Course -SEC 1	(Choose one from Group-G)	Internal Assessment			2

16. ELECTIVE COURSES

Courses are grouped (Group A to Group E) so as to include topics from Pure Chemistry (PC), Applied Chemistry (AC) and Industrial Components (IC) like Pharmaceutical Industries, Polymer labs courses for flexibility of choice by the stakeholders / institutions.

Semester I: Elective I and Elective II

Elective I to be chosen from **Group A** and **Elective II** to be chosen from **Group B**

Group A: (PC/AC/IC)

1. Pharmaceutical Chemistry
2. Nanomaterials and Nanotechnology

Group B (PC/AC/IC)

1. Electrochemistry
2. Molecular Spectroscopy

Semester II: Elective III & Elective IV

Elective III to be chosen from **Group C** and **Elective IV** to be chosen from **Group D**

Group C:**(PC/AC/IC)**

1. Medicinal Chemistry
2. Green Chemistry

Group D (PC/AC/IC)

1. Bioinorganic Chemistry
2. Material Science

Semester III: Elective V

Elective V to be chosen from **Group E**

Group E: (PC/AC/IC)

1. Pharmacognosy and Phytochemistry
2. Biomolecules and Heterocyclic compounds

17. SKILL ENHANCEMENT COURSES

Skill Enhancement Courses are chosen to keep in pace with the latest developments in the academic / industrial front and provides flexibility of choice by the stakeholders / institutions.

Group G (Skill Enhancement Courses) SEC: (Practical based paper)

- Computational Chemistry
- 3D printing in Chemistry
- Preparation of Consumer products
- Chemistry in everyday life

- Cosmetic Chemistry
- Origin lab
- Industrial Chemistry
- Research Tools and Techniques

18. TESTING PATTERN (25+75)

18.1 Internal Assessment

Theory Course: For theory courses, there shall be three tests conducted by the faculty concerned and the average of the best two can be taken as the Continuous Internal Assessment (CIA) for a maximum of 25 marks. The duration of each test shall be one / one and a half hour.

Computer Laboratory Courses: For Computer Laboratory Oriented Courses, there shall be two tests in Theory part and two tests in Laboratory part. Choose one best from Theory part and other best from the two Laboratory part. The average of the best two can be treated as the CIA for a maximum of 25 marks. The duration of each test shall be one / one and a half hour.

There is no improvement for CIA of both theory and laboratory, and, also for University End Semester Examination.

18.2 External Assessment

Written Examination: Theory Paper (Bloom's Taxonomy based)

Question Paper Model

Intended Learning Skills	**Maximum 75 Marks** **Passing Minimum: 50%** **Duration: Three Hours**
	Part –A (10x 2 = 20 Marks) Answer ALL questions **Each Question carries 2mark**
Memory Recall / Example/ Counter Example / Knowledge about the Concepts/ Understanding	Two questions from each UNIT
	Question 1 to Question 10
	Part – B (5 x 5 = 25 Marks) **Answer ALL questions** **Each questions carries 5 Marks**
Descriptions/ Application (Problems)	**Either-or -Type** Both parts of each question from the same UNIT
	Question 11(a) or 11(b) To **Question 15(a) or 15(b)**
	Part-C (3x 10 = 30 Marks) Answer any **THREE** questions **Each question carries 10 Marks**
Analysis /Synthesis / Evaluation	There shall be **FIVE** questions covering all the five units
	Question 16 to Question 20

Each question should carry the course outcome and cognitive level.
For instance,

1. [CO1: K2] Question xxxx
2. [CO3: K1] Question xxxx

19. DIFFERENT TYPES OF COURSES

(i) Core Courses

(ii) Elective Courses (ED within the Department Experts)

(iii) Skill Development Courses

(iv) Institution-Industry-Interaction (Industry aligned Courses)

Programmes /course work/ field study/ Modelling the Industry Problem/ Statistical Analysis /

Commerce-Industry related problems / MoU with Industry and the like activities.

20. SYLLABUS FOR M. Sc. CHEMISTRY

SEMESTER - I

<table>
<tr><td>Title of the Course</td><td colspan="7">ORGANIC REACTION MECHANISM - I</td></tr>
<tr><td>Paper No.</td><td colspan="7">Core I – CC1</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td rowspan="2">Credits</td><td rowspan="2">4</td><td rowspan="2">Course Code</td><td rowspan="2"></td></tr>
<tr><td>Semester</td><td>I</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="2">Lab Practice</td><td colspan="3">Total</td></tr>
<tr><td>4</td><td>1</td><td colspan="2">-</td><td colspan="3">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic concepts of organic chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the feasibility and the mechanism of various organic reactions.
To comprehend the techniques in the determination of reaction mechanisms.
To understand the concept of stereochemistry involved in organic compounds.
To correlate and appreciate the differences involved in the various types of organic reaction mechanisms.
To design feasible synthetic routes for the preparation of organic compounds.</td></tr>
<tr><td rowspan="2">Course Outline</td><td colspan="7">UNIT-I: Methods of Determination of Reaction Mechanism: Reaction intermediates, The transition state, Reaction coordinate diagrams, Thermodynamic and kinetic requirements of reactions, Hammond postulate. Methods of determining mechanism: Kinetic methods of determination: Rate law – Primary and secondary isotope effect. Non-Kinetic methods of determination: Testing and Trapping of intermediates, Isotopic labeling, Cross–over experiment, Product analysis and stereo chemical evidence.
Effect of structure on reactivity: Hammett and Taft equations. Linear free energy relationship, partial rate factor, substituent and reaction constants.</td></tr>
<tr><td colspan="7">UNIT-II: Aromatic and Aliphatic Electrophilic Substitution: Aromaticity: Aromaticity in benzenoid, non-benzenoid, heterocyclic compounds and annulenes.
Aromatic electrophilic substitution: Orientation and reactivity of di- and polysubstituted phenol, nitrobenzene and halobenzene. Reactions involving nitrogen electrophiles: nitration, nitrosation and diazonium coupling;</td></tr>
</table>

	Sulphur electrophiles: sulphonation; Halogen electrophiles: chlorination and bromination; Carbon electrophiles: Friedel-Crafts alkylation, acylation and arylation reactions. **Aliphatic electrophilic substitution Mechanisms**: SE2 and SEi, SE1-Mechanism and evidences.
	UNIT-III: **Aromatic and Aliphatic Nucleophilic Substitution:** **Aromatic nucleophilic substitution**: Mechanisms - S_NAr, S_N1 and Benzyne mechanisms - Evidences - Reactivity, Effect of structure, leaving group and attacking nucleophile. Reactions: Oxygen and Sulphur-nucleophiles, Bucherer and Rosenmund reactions, Von Richter, Sommelet-Hauser and Smiles rearrangements. **Aliphatic Nucleophilic Substitution**: S_N1, ion pair, S_N2 mechanisms and evidences. Aliphatic nucleophilic substitutions at an allylic carbon, aliphatic trigonal carbon and vinyl carbon. S_N1' S_N2' and S_Ni' mechanism and evidences, Swain- Scott, Grunwald-Winstein relationship - Ambident nucleophiles.
	UNIT-IV: Stereochemistry-I: Introduction to molecular symmetry and chirality – axis, plane, center, alternating axis of symmetry. Optical isomerism due to asymmetric and dissymmetric molecules with C, N, S based chiral centers. Optical purity, prochirality, enantiotopic and diastereotopic atoms, groups, faces, axial and planar chirality, chirality due to helical shape, methods of determining the configuration. Racemic modifications: Racemization by thermal, anion, cation, reversible formation, epimerization, mutarotation. D, L system, Cram's and Prelog's rules: R, S-notations, proR, proS, side phase and re phase Cahn-Ingold-Prelog rules, absolute and relative configurations. Configurations of allenes, spiranes, biphenyls, cyclooctene, helicene, binaphthyls, ansa and cyclophanic compounds, exo-cyclic alkylidene-cycloalkanes. Topicity and prostereoisomerism, chiral shift reagents and chiral solvating reagents. Criteria for optical purity: Resolution of racemic modifications, asymmetric transformations, asymmetric synthesis, destruction. Stereoselective and stereospecific synthesis.
	UNIT-V: Stereochemistry-II: Conformation and reactivity of acyclic

	systems, intramolecular rearrangements, neighbouring group participation, chemical consequence of conformational equilibrium - Curtin-Hammett Principle. Stability of five and six-membered rings: mono-, di- and polysubstituted cyclohexanes, conformation and reactivity in cyclohexane systems. Fused and bridged rings: bicyclic, poly cyclic systems, decalins and Brett's rule. Optical rotation and optical rotatory dispersion, conformational asymmetry, ORD curves, octant rule, configuration and conformation, Cotton effect, axial haloketone rule and determination of configuration.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved. (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. J. March and M. Smith, Advanced Organic Chemistry, 5th edition, John-Wiley and Sons.2001. 2. E. S. Gould, Mechanism and Structure in Organic Chemistry, Holt, Rinehart and Winston Inc., 1959. 3. P.S.Kalsi, Stereochemistry of carbon compounds, 8th edition, New Age International Publishers, 2015. 4. P. Y. Bruice, Organic Chemistry, 7th edn, Prentice Hall, 2013. 5. J.Clayden, N. Greeves, S. Warren, Organic Compounds, 2nd edition, Oxford University Press, 2014.
Reference Books	1. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part-A and B, 5th edition, Kluwer Academic / Plenum Publishers, 2007. 2. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001. 3. N.S. Isaacs, Physical Organic Chemistry, ELBS, Longman, UK, 1987. 4. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata-McGraw Hill, 2000. 5. I. L. Finar, Organic chemistry, Vol-1 & 2, 6th edition, Pearson Education Asia, 2004.
Website and e-learning source	1.https://sites.google.com/site/chemistryebookscollection02/home/organic-chemistry/organic 2. https://www.organic-chemistry.org/
Course Outcomes (for Mapping with POs and PSOs) Students will be able	

CO1: To recall the basic principles of organic chemistry.
CO2: To understand the formation and detection of reaction intermediates of organic reactions.
CO3: To predict the reaction mechanism of organic reactions and stereochemistry of organic compounds.
CO4: To apply the principles of kinetic and non-kinetic methods to determine the mechanism of reactions.
CO5: To design and synthesize new organic compounds by correlating the stereochemistry of organic compounds.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

Strong – 3, Medium-2, Low-1

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

Methods of Evaluation		
Internal Evaluation	Continuous Internal Assessment Test	25 Marks
	Assignments	
	Seminars	
	Attendance and Class Participation	
External Evaluation	End Semester Examination	75 Marks
	Total	100 Marks
Methods of Assessment		

Recall (K1)	Simple definitions, MCQ, Recall steps, Concept definitions.
Understand/ Comprehend (K2)	MCQ, True/False, Short essays, Concept explanations, short summary or overview.
Application (K3)	Suggest idea/concept with examples, suggest formulae, solve problems, Observe, Explain.
Analyze (K4)	Problem-solving questions, finish a procedure in many steps, Differentiate between various ideas, Map knowledge.
Evaluate (K5)	Longer essay/ Evaluation essay, Critique or justify with pros and cons.
Create (K6)	Check knowledge in specific or offbeat situations, Discussion, Debating or Presentations.

In order to avoid pull the score down of each PO, it is suggested that the usage L-Low (1) to the minimum.
The S, M, L is based on the course outcome. The mapping is based on the revised Bloom's Taxonomy Verbs used to describe your course outcome.

- Remember and Understanding – Lower level
- Apply and Analyze – Medium Level
- Evaluate and Create – Strong Level

<table>
<tr><td>Title of the Course</td><td colspan="7">STRUCTURE AND BONDING IN INORGANIC COMPOUNDS</td></tr>
<tr><td>Paper No.</td><td colspan="7">Core II – CC2</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td>Credits</td><td>4</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>I</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>4</td><td>1</td><td colspan="3">-</td><td colspan="2">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic concepts of Inorganic Chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To determine the structural properties of main group compounds and clusters.
To gain fundamental knowledge on the structural aspects of ionic crystals.
To understand structures and bonding in inorganic polymers and metal clusters.
To study the effect of point defects and line defects in ionic crystals.
To evaluate the structural aspects of solids.</td></tr>
<tr><td rowspan="2">Course Outline</td><td colspan="7">UNIT I - CHEMICAL BONDING
Valence Bond theory: Lewis structure – Concepts and VB theory of H_2 molecule - Stereochemistry of hybrid orbitals – Calculation of s and p characters of equivalence and nonequivalence of hybrid orbitals - VSEPR theory.
M.O. theory – Linear combination of Atomic orbitals (s – s, s – p, d – p, p – p and d –d overlapping) – σ , π ,δ and quadruple bond. – M.O. diagrams of hetero nuclear diatomic molecules (CO, NO, HF) and triatomic molecules (BeH_2, H_2O, CO_2) – Walsh diagrams – Structure and hybridization - Bents rule and apicophilicity.
Ionic Bond: Lattice energy - Born-Lande equation, Born Haber cycle and Kapustinskii equation.</td></tr>
<tr><td colspan="7">UNIT-II: Structure of main group compounds and clusters: Structure of silicates - applications of Pauling’s rule of electrovalence - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three-dimensional silicates. Structure of silicones, Structural and bonding features of B-N, S-N and P-N compounds; Poly acids – types, examples and structures; Borane cluster: Structural features of closo, nido, arachano and klado; carboranes, hetero and metalloboranes; Wade’s rule to predict the tructure of borane cluster; main group clusters –zintl ions.</td></tr>
</table>

	UNIT-III: Solid state chemistry – I: Ionic crystals: Packing of ions in simple, hexagonal and cubic close packing, voids in crystal lattice, Radius ratio, Crystal systems and Bravais lattices, Symmetry operations in crystals, glide planes and screw axis; point group and space group. X-ray diffraction technique: Bragg's law, Powder diffraction method – Principle and Instrumentation.
	UNIT-IV: Solid state chemistry – II: Structural features of the crystal systems: Rock salt, zinc blende & wurtzite, fluorite and anti-fluorite, rutile and anatase, cadmium iodide and nickel arsenide; Spinels -normal and inverse types and perovskite structures. Crystal Growth methods: From melt and solution (hydrothermal, sol-gel methods) – principles and examples.
	UNIT-V: Band theory and defects in solids Band theory – features and its application of conductors, insulators and semiconductors, Intrinsic and extrinsic semiconductors; Defects in crystals – point defects (Schottky, Frenkel, metal excess and metal deficient) and their effect on the electrical and optical property; Linear defects and its effects due to dislocations and colour centers.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. A R West, Solid state Chemistry and its applications, 2ndEdition (Students Edition), John Wiley & Sons Ltd., 2014. 2. A K Bhagi and G R Chatwal, A textbook of inorganic polymers, Himalaya Publishing House, 2001. 3. L Smart, E Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2012. 4. K. F. Purcell and J. C. Kotz, Inorganic Chemistry; W.B. Saunders company: Philadelphia, 1977. 5. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry; 4th ed.; Harper and Row: NewYork, 1983.

Reference Books	1. D. E. Douglas, D.H. McDaniel and J. J. Alexander, Concepts and Models in Inorganic Chemistry, 3rd Ed, 1994. 2. R J D Tilley, Understanding Solids - The Science of Materials, 2nd edition, Wiley Publication, 2013. 3. C N R Rao and J Gopalakrishnan, New Directions in Solid State Chemistry, 2nd Edition, Cambridge University Press, 199. 4. T. Moeller, Inorganic Chemistry, A Modern Introduction; John Wiley: New York, 1982. 5. D. F. Shriver, P. W. Atkins and C.H. Langford; Inorganic Chemistry; 3rd ed.; Oxford University Press: London, 2001.
Website and e-learning source	https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video_galleries/lecture-videos/

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able

CO1: To predict the geometry of main group compounds and clusters.

CO2: To explain about the packing of ions in crystals and apply the radius ratio rule to predict the coordination number of cations.

CO3: To understand the various types of ionic crystal systems and analyze their structural features.

CO4: To explain the crystal growth methods.

CO5: To understand the various types of defects in crystals.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">ORGANIC CHEMISTRY PRACTICAL-I</td></tr>
<tr><td>Paper No.</td><td colspan="7">Core III - CC3</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td>Credits</td><td>3</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>I</td><td colspan="4"></td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>-</td><td>1</td><td colspan="3">4</td><td colspan="2">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic concepts of organic chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the concept of separation, qualitative analysis and preparation of organic compounds.
To develop analytical skill in the handling of chemical reagents for separation of binary and ternary organic mixtures.
To analyze the separated organic components systematically and derivative them suitably.</td></tr>
<tr><td>Course Outline</td><td colspan="7">A. Qualitative analysis of Organic mixture (atleast six two component mixtures):
• Separation of organic mixtures
• Elemental analysis
• Functional group(s) identification
• Preparation of derivatives
• Physical properties determination (melting point and boiling point) for both components and their derivatives.
Analysis may be performed in micro (or) macro scale depending upon the conditions of the laboratory.
B. For Class work:
Three component mixtures (Separation)</td></tr>
<tr><td>Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)</td><td colspan="7">Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved
(To be discussed during the Tutorial hours)</td></tr>
<tr><td>Skills acquired from this course</td><td colspan="7">Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.</td></tr>
<tr><td>Recommended Text</td><td colspan="7">1. A.I. Vogel, Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, 2011.
2. K. Bansal Raj, Laboratory Manual of Organic Chemistry, New Age International, 2009.
3. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, Basic Principles of Practical Chemistry, Sultan Chand & Sons, 2004.
4. V.K. Ahluwalia, and R. Aggarwal, Comprehensive Practical</td></tr>
</table>

	Organic Chemistry, UniversitiesPress, 2004
Reference Books	1. R.G. Engel, D.L. Pavia, G.M. Lampman and G.S. Kriz, A Microscale approach to Organic Laboratory, 5th edition, Paperback – International Edition, 2012. 2. P.B. Cranwell, L.M. Harwood, and C. J. Moody, Experimental Organic Chemistry, 3rd edn, Wiley-Blackwell, 2017. 3. J. Leonard, B. Lygo and G. Procter, Advanced Practical Organic Chemistry, 3rd edn, CRC Press, 2013.
Website and e-learning source	https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video_galleries/lecture-videos/

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:
CO1: To explain the basic separation procedures of organic mixtures.
CO2: To select the separation methods to separate the organic mixtures.
CO3: To classify the functional groups using systematic procedure.
CO4: To determine the physical properties of organic compounds.
CO5: To analyze the separated organic components systematically and derivative them suitably.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	S	S	S	S	M	S	S	S	S	M
CO 2	M	S	S	S	S	M	S	S	S	S
CO 3	S	S	M	S	S	S	S	M	S	S
CO 4	M	S	S	S	S	M	S	S	S	S
CO 5	M	S	M	S	S	M	S	M	S	S

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 – Low

<table>
<tr><td>Title of the Course</td><td colspan="7">PHYSICAL CHEMISTRY PRACTICAL</td></tr>
<tr><td>Paper No.</td><td colspan="7">Core IV- CC4</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td rowspan="2">Credits</td><td rowspan="2">3</td><td rowspan="2">Course Code</td><td rowspan="2"></td></tr>
<tr><td>Semester</td><td>I</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>-</td><td>1</td><td colspan="3">4</td><td colspan="2">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of physical chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the principle of conductivity experiments through conductometric titrations.
To evaluate the order of the reaction, temperature coefficient and activation energy of the reaction by following pseudo first order kinetics.
To construct the phase diagram of two component system forming congruent melting solid and find its eutectic temperatures and compositions.</td></tr>
<tr><td rowspan="3">Course Outline</td><td colspan="7">UNIT-I: Conductivity Experiments
1. Determination of equivalent conductance of a strong electrolyte & the verification of DHO equation.
2. Verification of Ostwald’s Dilution Law & Determination of pKa of a weak acid.
3. Verification of Kohlrausch’s Law for weak electrolytes.
4. Determination of the equivalent conductance of a weak acid at different concentrations and verifying Ostwald dilution law.
5. Calculation of the dissociation constant of the acid. Determination of the equivalent conductance of a strong electrolyte at different concentrations and examining the validity of the Onsager’s theory as limiting law at high dilutions.
6. Conductometric titration of a mixture of HCl and CH_3COOH Vs NaOH.
7. Conductometric titration of NH_4Cl Vs NaOH.
8. Conductometric titration of CH_3COONa Vs HCl.</td></tr>
<tr><td colspan="7">UNIT-II: Kinetics
1. Study the kinetics of acid hydrolysis of an ester; determine the temperature coefficient and also the activation energy of the reaction.
2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half-life method and determine the order with respect to iodine and acetone.</td></tr>
<tr><td colspan="7">UNIT-III: Phase diagram
Construction of phase diagram for a simple binary system
1. Naphthalene-phenanthrene
2. Benzophenone- diphenyl amine.</td></tr>
<tr><td>Extended</td><td colspan="7">Questions related to the above topics, from various competitive</td></tr>
</table>

Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. B. Viswanathan and P.S.Raghavan, Practical Physical Chemistry, Viva Books, New Delhi, 2009. 2. Sundaram, Krishnan, Raghavan, Practical Chemistry (Part II), S. Viswanathan Co. Pvt., 1996. 3. V.D. Athawale and Parul Mathur, Experimental Physical Chemistry, New Age International (P) Ltd., New Delhi, 2008. 4. E.G. Lewers, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Ed., Springer, New York, 2011.
Reference Books	1. J.B.Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001. 2.G.W.Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th edition, McGraw Hill, 2009. 3. J.N.Gurthu and R. Kapoor, Advanced Experimental Chemistry, S. Chand and Co., 1987. 4. Shailendra K Sinha, Physical Chemistry: A laboratory Manual, Narosa Publishing House Pvt, Ltd., New Delhi, 2014. 5. F. Jensen, Introduction to Computational Chemistry, 3rd Ed., Wiley-Blackwell.
Website and e-learning source	https://web.iitd.ac.in/~nkurur/2015-16/Isem/cmp511/lab_handout_new.pdf

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To recall the principles associated with various physical chemistry experiments.

CO2: To explain the principles of conductometric titrations and estimate the strength of solutions.

CO3: To observe and record systematically the readings in all the experiments.

CO4: To calculate and process the experimentally measured values and compare with graphical data.

CO5: To interpret the experimental data scientifically to improve students' efficiency for societal developments.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 – Low

Level of Correlation between PSO's and CO's

CO /PO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to Pos	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 – Low

<table>
<tr><td>Title of the Course</td><td colspan="7">PHARMACEUTICAL CHEMISTRY</td></tr>
<tr><td>Paper No.</td><td colspan="7">Elective I – EC1</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Elective</td><td>Year</td><td>I</td><td>Credits</td><td>3</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>I</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>4</td><td>1</td><td colspan="3">-</td><td colspan="2">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge on drugs and doses</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the advanced concepts of pharmaceutical chemistry.
To recall the principle and biological functions of various drugs.
To train the students to know the importance as well the consequences of various drugs.
To familiarize on the drug dosage and its structural activities.</td></tr>
<tr><td rowspan="3">Course Outline</td><td colspan="7">UNIT-I: Physical properties in Pharmaceuticals: Physical properties of drug molecule: physical properties. Refractive index- Definition, explanation, formula, importance, determination, specific & molar refraction. Optical activity\rotation- monochromatic & polychromatic light, optical activity, angle of rotation, specific rotation examples, measurement of optical activity. Dielectric constant & Induced Polarization- Dielectric constant explanation & determination. Rheology of pharmaceutical systems: Introduction, Definition, Applications, concept of viscosity, Newton’s law of flow, Kinematic, Relative, Specific, Reduced & Intrinsic viscosity. Newtonian system, non-Newtonian system- Plastic flow, Pseudoplastic flow, Dilatant flow. Viscosity measurements- selection of viscometer for Newtonian and non-Newtonian system.</td></tr>
<tr><td colspan="7">UNIT-II: Isotopic Dilution analysis: principle and applications, Neutron activation analysis: Principle, advantages and limitations, Scintillation counters: Body scanning. Introduction to radiopharmaceuticals. Properties of various types of radiopharmaceuticals, Radiopharmaceuticals as diagnostics, as therapeutics, for research and sterilization. Physico Chemical Properties and drug action. Physico chemical properties of drugs (a) Partition coefficient, (b) solubility (c) surface activity, (d) degree of ionization.</td></tr>
<tr><td colspan="7">UNIT-III: Drug dosage and product development: Introduction to Drug Dosage Forms & Drug Delivery system – Definition of Common terms. Drug Regulation and control, pharmacopoeias formularies,</td></tr>
</table>

	sources of drug, drug nomenclature, routes of administration of drug products, need for a dosage form, classification of dosage forms.
	UNIT-IV: Development of new drugs: Introduction, procedure followed in drug design, the research for lead compounds, molecular modification of lead compounds. Structure-Activity Relationship (SAR): Factors effecting bioactivity, resonance, inductive effect, isosterism, bioisosterism, spatial considerations, biological properties of simple functional groups, theories of drug activity, occupancy theory, rate theory, induced-fit theory. Quantitative structure activity relationship (QSAR): Development of QSAR, drug receptor interactions, the additivity of group contributions, physico-chemical parameters, lipophilicity parameters, electronic parameter, ionization constants, steric parameters, chelation parameters, redox potential, indicator-variables.
	UNIT-V: Computers in Pharmaceutical Chemistry: Need of computers for chemistry. Computers for Analytical Chemists-Molecular Docking – Selection of binding protein – RCSB – Druglikeness of the ligand – ADMET properties – Detection using online servers – AutoDock Vina – Methods and Result analysis – Visualization of the Ligand-Protein interaction.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. Physical Chemistry- Bahl and Tuli. 2. Text Book of Physical Pharmaceutics, IInd edition, Vallabh Prakashan-. C.V.S. Subramanyam. 3. Medicinal Chemistry (Organic Pharmaceutical Chemistry), G.R Chatwal, Himalaya Publishing house. 4. Instrumental method of Analysis: Hubert H, Willard, 7th edition. 5. Textbook of Pharmaceutical Chemistry by, Jayshree Ghosh, S. Chand & company Ltd. Pharmaceutical Chemistry by Dr. S. Lakshmi, Sultan chand & Sons.

Reference Books	1. Computers in chemistry, K.V. Raman, Tata Mc.Graw-Hill, 1993. 2. Computers for Chemists, S.K Pundir, Anshu bansal, A pragate prakashan., 2 nd edition, New age international (P) limited, New Delhi. 3. Physical Pharmacy and Pharmaceutical Sciences by Martins, Patrick J. Sinko, Lippincott. William and Wilkins. 4. Cooper and Gunn's Tutorial Pharmacy ,6th edition by S.J. Carter, CBS Publisher Ltd. 5. Ansels pharmaceutical Dosage forms and Drug Delivery System by Allen Popvich and Ansel, Indian edition-B.I. Publication Pvt. Ltd.
Website and e-learning source	https://www.ncbi.nlm.nih.gov/books/NBK482447/ https://training.seer.cancer.gov/treatment/chemotherapy/types.html

Course Learning Outcomes (for Mapping with POs and PSOs)
Students will be able:

CO1: To identify the suitable drugs for various diseases.
CO2: To apply the principles of various drug action and drug design.
CO3: To acquire the knowledge on product development based on SAR.
CO4: To apply the knowledge on applications of computers in chemistry.
CO5: To synthesize new drugs after understanding the concepts SAR.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	S	S	S	S	M	S	S	S	S	M
CO 2	M	S	S	S	S	M	S	S	S	S
CO 3	S	S	M	S	S	S	S	M	S	S
CO 4	M	S	S	S	S	M	S	S	S	S
CO 5	M	S	M	S	S	M	S	M	S	S

3 – Strong, 2 – Medium, 1 - Low

Level Of Correlation Between PSO's And CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">NANO MATERIALS AND NANO TECHNOLOGY</td></tr>
<tr><td>Paper No.</td><td colspan="7">Elective I – EC1</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Elective</td><td>Year</td><td>I</td><td rowspan="2">Credits</td><td rowspan="2">3</td><td rowspan="2">Course Code</td><td rowspan="2"></td></tr>
<tr><td>Semester</td><td>I</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>4</td><td>1</td><td colspan="3">-</td><td colspan="2">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of crystallography and material science</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the concept of nano materials and nano technology.
To understand the various types of nano materials and their properties.
To understand the applications of synthetically important nano materials.
To correlate the characteristics of various nano materials synthesized by new technologies.
To design synthetic routes for synthetically used new nano materials.</td></tr>
<tr><td>Course Outline</td><td colspan="7">UNIT-I: Introduction of nanomaterials and nanotechnologies: Introduction-role of size, classification-0D, 1D, 2D, 3D. consolidation of Nano powders. Features of nanostructures, Background of nanostructures. Techniques of synthesis of nanomaterials- Bottom –Up, Top–Down, Tools of the nanoscience. Applications of nanomaterials and technologies.</td></tr>
<tr><td></td><td colspan="7">UNIT-II: Synthetic Methods: Bonding and structure of the nanomaterials, Predicting the Type of Bonding in a Substance crystal structure. Metallic nanoparticles, Surfaces of Materials, Nanoparticle Size and Properties. Synthesis- Physical and chemical methods - inert gas condensation, arc discharge, laser ablation, sol-gel, solvothermal and hydrothermal-CVD-types, metallo organic, plasma enhanced, and low-pressure CVD. Microwave assisted and electrochemical synthesis.</td></tr>
<tr><td></td><td colspan="7">UNIT-III: Mechanical Properties of Nanomaterials: Mechanical properties of materials, theories relevant to mechanical properties. Techniques to study mechanical properties of nanomaterials, adhesion and friction, thermal properties of nanomaterials
Nanoparticles: gold and silver, metal oxides: silica, iron oxide and alumina - synthesis and properties.</td></tr>
<tr><td></td><td colspan="7">UNIT-IV: Electrical Properties of Nanomaterials: Electrical properties, Conductivity and Resistivity, Classification of Materials</td></tr>
</table>

	based on Conductivity, magnetic properties, electronic properties of materials. Classification of magnetic phenomena. Semiconductor materials – classification-Ge, Si, GaAs, SiC, GaN, GaP, CdS,PbS. Identification of materials as p and n –type semiconductor-Hall effect - quantum and anomalous, Hall voltage - interpretation of charge carrier density. Applications of semiconductors: p-n junction as transistors and rectifiers, photovoltaic and photogalvanic cell.
	UNIT-V: Nano Composites: Nano thin films, nanocomposites. Application of nanoparticles in different fields. Core-shell nanoparticles - types, synthesis, and properties. Nanocomposites - metal- ceramic- and polymer-matrix composites-applications. Characterization – SEM, TEM and AFM - principle, instrumentation and applications.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. S.Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016. 2. Arumugam, Materials Science, Anuradha Publications,2007. 3. Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010 4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012. 5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.
Reference Books	1. S.Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016. 2. Arumugam, Materials Science, Anuradha Publications,2007. 3. Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010 4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012. 5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction

	to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.
Website and e-learning source	1. http://xrayweb.chem.ou.edu/notes/symmetry.html. 2. http://www.uptti.ac.in/classroom-content/data/unit%20cell.pdf.

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:
CO1: To explain methods of fabricating nanostructures.
CO2: To relate the unique properties of nanomaterials to reduce dimensionality of the material.
CO3: To describe tools for properties of nanostructures.
CO4: To discuss applications of nanomaterials.
CO5: To understand the health and safety related to nanomaterial.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	S	S	S	S	M	S	S	S	S	M
CO 2	M	S	S	S	S	M	S	S	S	S
CO 3	S	S	M	S	S	S	S	M	S	S
CO 4	M	S	S	S	S	M	S	S	S	S
CO 5	M	S	M	S	S	M	S	M	S	S

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">ELECTROCHEMISTRY</td></tr>
<tr><td>Paper No.</td><td colspan="7">Elective II - EC2</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Elective</td><td>Year</td><td>I</td><td rowspan="2">Credits</td><td rowspan="2">3</td><td rowspan="2">Course Code</td><td rowspan="2"></td></tr>
<tr><td>Semester</td><td>I</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>4</td><td>1</td><td colspan="3">-</td><td colspan="2">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of electrochemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the behavior of electrolytes in terms of conductance, ionic atmosphere, interactions.
To familiarize the structure of the electrical double layer of different models.
To compare electrodes between current density and over potential.
To discuss the mechanism of electrochemical reactions.
To highlight the different types of over voltages and its applications in electroanalytical techniques.</td></tr>
<tr><td rowspan="3">Course Outline</td><td colspan="7">UNIT-I: Ionics: Arrhenius theory -limitations, Van’t Hoff factor and its relation to colligative properties. Deviation from ideal behavior. Ionic activity, mean ionic activity and mean ionic activity coefficient-concept of ionic strength, Debye Huckel theory of strong electrolytes, activity coefficient of strong electrolytes Determination of activity coefficient ion - solvent and ion-ion interactions. Derivation of Debye-Huckel limiting law at appreciable concentration of electrolytes modifications and applications. Electrolytic conduction-Debye-Huckel Onsager treatment of strong electrolyte-qualitative and quantitative verification and limitations.</td></tr>
<tr><td colspan="7">UNIT-II: Electrode-electrolyte interface: Interfacial phenomena - Evidences for electrical double layer, polarizable and non-polarizable interfaces, Electrocapillary phenomena - Lippmann equation electro capillary curves. Electro-kinetic phenomena electro-osmosis, electrophoresis, streaming and sedimentation potentials, colloidal and poly electrolytes. Structure of double layer: Helmholtz -Perrin, Guoy-Chapman and Stern models of electrical double layer. Zeta potential and potential at zero charge. Applications and limitations.</td></tr>
<tr><td colspan="7">UNIT-III: Electrodics of Elementary Electrode Reactions: Behavior of electrodes: Standard electrodes and electrodes at equilibrium. Anodic and Cathodic currents, condition for the discharge of ions. Nernst</td></tr>
</table>

	equation, polarizable and non-polarizable electrodes. Model of three electrode system, over potential. Rate of electro chemical reactions: Rates of simple elementary reactions. Butler-Volmer equation and Tafel equation-significance of exchange current density, net current density and symmetry factor. Low and high field approximations. symmetry factor and transfer coefficient Tafel equations and Tafel plots.
	UNIT-IV: Electrodics of Multistep Multi Electron System: Rates of multi-step electrode reactions. Rate determining step, electrode polarization and depolarization. Transfer coefficients, its significance and determination, Stoichiometric number. Reduction of I^{3-}, Fe^{2+} and dissolution of Fe to Fe^{2+}. Overvoltage - Chemical and electro chemical, Phase, activation and concentration over potentials. Evolution of oxygen and hydrogen at different pH. Pourbiax and Evan's diagrams.
	UNIT-V: Concentration Polarization, Batteries and Fuel cells: Modes of Transport of electro active species - Diffusion, migration and hydrodynamic modes. Role of supporting electrolytes. Polarography-principle and applications. Cyclic voltammetry- anodic and cathodic stripping voltammetry and differential pulse voltammetry. Sodium and lithium-ion batteries and redox flow batteries. Energy production systems: Fuel Cells: classification, alkaline fuel cells, phosphoric acid fuel cells, high temperature fuel cells.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. D. R. Crow, Principles and applications of electrochemistry, 4thedition, Chapman & Hall/CRC, 2014. 2. J. Rajaram and J.C. Kuriakose, Kinetics and Mechanism of chemical transformations Macmillan India Ltd., New Delhi, 2011. 3. S. Glasstone, Electro chemistry, Affiliated East-West Press, Pvt., Ltd., New Delhi, 2008.

	4. B. Viswanathan, S. Sundaram, R. Venkataraman, K. Rengarajan and P.S. Raghavan, Electrochemistry-Principles and applications, S. Viswanathan Printers, Chennai,2007. 5. Joseph Wang, Analytical Electrochemistry, 2nd edition, Wiley, 2004.
Reference Books	1. J.O.M. Bockris and A.K.N. Reddy, Modern Electro chemistry, vol.1 and 2B, Springer, Plenum Press, New York, 2008. 2. J.O.M. Bockris, A.K.N. Reddy and M.G. Aldeco Morden Electro chemistry, vol. 2A, Springer, Plenum Press, New York, 2008. 3. Philip H. Rieger, Electrochemistry, 2nd edition, Springer, New York, 2010. 4. L.I. Antropov, Theoretical electrochemistry, Mir Publishers, 1977. 5. K.L. Kapoor, A Text book of Physical chemistry, volume-3, Macmillan, 2001.
Website and e-learning source	1. https://www.pdfdrive.com/modern-electrochemistry-e34333229.

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To understand the behaviour of electrolytes in solution and compare the structures of electrical double layer of different models.

CO2: To predict the kinetics of electrode reactions applying Butler-Volmer and Tafel equations

CO3: To study the mechanism of multi- step electrode reactions.

CO4: To discuss the theories of electrolytes, electrical double layer, electrodics and activity coefficient of electrolytes

CO5: To have knowledge on storage devices and electrochemical reaction mechanism.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">MOLECULAR SPECTROSCOPY</td></tr>
<tr><td>Paper No.</td><td colspan="7">Elective II – EC2</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Elective</td><td>Year</td><td>I</td><td rowspan="2">Credits</td><td rowspan="2">3</td><td rowspan="2">Course Code</td><td rowspan="2"></td></tr>
<tr><td>Semester</td><td>I</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>4</td><td>1</td><td colspan="3">-</td><td colspan="2">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of spectroscopy</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the influence of rotation and vibrations on the spectra of the polyatomic molecules.
To study the principle of Raman spectroscopy, ESR spectroscopy and fragmentation patterns in Mass spectroscopy.
To highlight the significance of Franck-Condon principle to interpret the selection rule, intensity and types of electronic transitions.
To interpret the first and second order NMR spectra in terms of splitting and coupling patterns using correlation techniques such as COSY, HETCOR, NOESY.
To carry out the structural elucidation of molecules using different spectral techniques.</td></tr>
<tr><td rowspan="2">Course Outline</td><td colspan="7">UNIT-I: Rotational and Raman Spectroscopy: Rotational spectra of diatomic and polyatomic molecules. Intensities of rotational spectral lines, effect of isotopic substitution. Non-rigid rotators. Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and asymmetric top molecules, Stokes and anti-Stokes lines. Vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure-Q and S branches, Polarization of Raman scattered photons.</td></tr>
<tr><td colspan="7">UNIT-II: Vibrational Spectroscopy: Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution. Diatomic vibrating rotor, vibrational-rotational spectra of diatomic molecules, P, R branches, breakdown of the Born-Oppenheimer approximation. Vibrations of polyatomic molecules – symmetry properties, overtone and combination frequencies. Influence of rotation</td></tr>
</table>

	on vibrational spectra of polyatomic molecule, P, Q, R branches, parallel and perpendicular vibrations of linear and symmetric top molecules.
	UNIT-III: Electronic spectroscopy: Electronic Spectroscopy: Electronic spectroscopy of diatomic molecules, Frank-Condon principle, dissociation and predissociation spectra. $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions and their selection rules. Photoelectron Spectroscopy: Basic principles, photoelectron spectra of simple molecules, Xray photoelectron spectroscopy (XPS). Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems.
	UNIT-IV: NMR and Mass Spectrometry: Chemical shift, Factors influencing chemical shifts: electronegativity and electrostatic effects; Mechanism of shielding and deshielding. Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra. Spin-spin interactions: Homonuclear coupling interactions - AX, AX2, AB types. Vicinal, germinal and long-range coupling-spin decoupling. Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities. ^{13}C NMR and structural correlations – DEPT. Brief introduction to 2D NMR – COSY, NOESY and HETCOR. Introduction to ^{31}P, ^{19}F NMR. Mass Spectrometry: **Mass Spectrometry:** Ionization techniques- Electron ionization (EI), chemical ionization (CI), desorption ionization (FAB/MALDI), electrospray ionization (ESI), isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution. Effect of isotopes on the appearance of mass spectrum. Structural elucidation of organic compounds by combined spectral techniques.
	UNIT-V: ESR and Mossbauer Spectroscopy: ESR spectroscopy Characteristic features of ESR spectra, line shapes and line widths; ESR spectrometer. The g value and the hyperfine coupling parameter (A), origin of hyperfine interaction. Interpretation of ESR spectra and

	structure elucidation of organic radicals using ESR spectroscopy; Spin orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals. ESR spectra of magnetically dilute samples. Principle of Mossbauer spectroscopy: Doppler shift, recoil energy. Isomer shift, quadrupole splitting, magnetic interactions. Applications: Mossbauer spectra of high and low-spin Fe and Sn compounds.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw Hill, New Delhi, 2000. 2. R. M. Silverstein and F. X. Webster, *Spectroscopic Identification of Organic Compounds*, 6th Ed., John Wiley & Sons, New York, 2003. 3. W. Kemp, *Applications of Spectroscopy*, English Language Book Society, 1987. 4. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 4th Ed., Tata McGraw-Hill Publishing Company, New Delhi, 1988. 5. R. S. Drago, *Physical Methods in Chemistry*; Saunders: Philadelphia, 1992.
Reference Books	1. P.W. Atkins and J. de Paula, *Physical Chemistry*, 7th Ed., Oxford University Press, Oxford, 2002. 2. I. N. Levine, *Molecular Spectroscopy*, John Wiley & Sons, New York, 1974. 3. A. Rahman, *Nuclear Magnetic Resonance-Basic Principles*, Springer-Verlag, New York,1986. 4. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and coordination Compounds*, PartB: 5th ed., John Wiley& Sons Inc., New York, 1997. 5. J. A. Weil, J. R. Bolton and J. E. Wertz, *Electron Paramagnetic Resonance*; Wiley Interscience, 1994.
Website and e-learning source	1. https://onlinecourses.nptel.ac.in/noc20_cy08/preview 2. https://www.digimat.in/nptel/courses/video/104106122/L14.html

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To understand the importance of rotational and Raman spectroscopy.

CO2: To apply the vibrational spectroscopic techniques to diatomic and polyatomic molecules.

CO3: To evaluate different electronic spectra of simple molecules using electronic spectroscopy.

CO4: To outline the NMR, ^{13}C NMR, 2D NMR – COSY, NOESY, Introduction to ^{31}P, ^{19}F NMR and ESR spectroscopic techniques.

CO5: To develop the knowledge on principle, instrumentation and structural elucidation of simple molecules using Mass Spectrometry, EPR and Mossbauer Spectroscopy techniques.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

SEMESTER - II

<table>
<tr><td>Title of the Course</td><td colspan="7">ORGANIC REACTION MECHANISM - II</td></tr>
<tr><td>Paper No.</td><td colspan="7">Core V – CC5</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td>Credits</td><td>4</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>II</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>4</td><td>1</td><td colspan="3">-</td><td colspan="2">5</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of organic chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the mechanism involved in various types of organic reactions with evidences.
To understand the applications of synthetically important reagents.
To design synthetic routes for synthetically used organic reactions.</td></tr>
<tr><td rowspan="2">Course Outline</td><td colspan="7">UNIT-I: Elimination and Free Radical Reactions: Mechanisms: E2, E1, and E1cB mechanisms. Syn- and anti-eliminations. Orientation of the double bond: Hoffmann and Saytzeff rules. Reactivity: Effect of substrate, attacking bases, leaving group and medium. Stereochemistry of eliminations in acyclic and cyclic systems, pyrolytic elimination.
Long lived and short-lived radicals – Production of radicals by thermal and photochemical reactions, Detection and stability of radicals, characteristics of free radicals, Reactions of radicals: polymerization, addition, halogenations, aromatic substitutions, rearrangements. Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent.</td></tr>
<tr><td colspan="7">UNIT-II: Oxidation and Reduction Reactions: Mechanisms: Direct electron transfer, hydride transfer, hydrogen transfer, displacement, addition-elimination, oxidative and reductive coupling reactions.
Mechanism of oxidation reactions: Dehydrogenation by quinones, selenium dioxides, ferricyanide, mercuric acetate, lead tetraacetate, osmium tetroxide, Reactions involving cleavage of C-C bonds - cleavage of double bonds, oxidative decarboxylation, allylic oxidation, oxidation by chromium trioxide-pyridine, DMSO-Oxalyl chloride (Swern oxidation) and Corey-</td></tr>
</table>

	Kim oxidation, dimethyl sulphoxide- dicyclohexyl carbodiimide (DMSO-DCCD). **Mechanism of reduction reactions:** Wolff-Kishner, Clemmenson, Rosenmund, reduction with Trialkyl and triphenyltin hydrides, Homogeneous hydrogenation, Hydroboration with cyclic systems, MPV and Bouveault-Blanc reduction.
	UNIT-III: Rearrangements: **Rearrangements to electron deficient carbon:** Pinacol-pinacolone and semi-pinacolone rearrangements - applications and stereochemistry, Wagner-Meerwein, Demjanov, Dienone-phenol, Benzilic acid and Wolff rearrangements. **Rearrangements to electron deficient nitrogen:** Hofmann, Curtius, Schmidt, Lossen, Beckmann and abnormal Beckmann rearrangements. **Rearrangements to electron deficient oxygen:** Baeyer-Villiger oxidation and Dakin rearrangements. **Rearrangements to electron rich atom:** Favorskii, Quasi-Favorskii, Stevens, [1,2]-Wittig and [2,3]-Wittig rearrangements. Fries and Photo Fries rearrangement. **Intramolecular rearrangements:** Claisen, abnormal Claisen, Cope, oxy-Cope and Benzidine rearrangements.
	UNIT-IV: Addition to Carbon Multiple Bonds: **Mechanisms: Addition to carbon-carbon multiple bonds:** Addition reactions involving electrophiles, nucleophiles, free radicals, carbenes and cyclic mechanisms-Orientation and reactivity, hydrogenation of double and triple bonds, Michael reaction, addition of oxygen and Nitrogen **Addition to carbon-hetero atom multiple bonds:** Mannich reaction, acids, esters, nitrites, addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction, Prins reaction. Stereochemical aspects of addition reactions. Mechanism of condensation reactions involving enolates –Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.
	UNIT-V: Reagents and Modern Synthetic Reactions: Lithium diisopropylamine (LDA), Sodium cyanoborohydride ($NaBH_3CN$),

	meta-Chloroperbenzoic acid (m-CPBA), Dimethyl aminiopyridine (DMAP), n-Bu_3SnD, Triethylamine (TEA), Diethylazodicarboxylate (DEAD), *N*-bromosuccinimide (NBS), Trifluoroacetic acid (TFA), Phenyl trimethyl ammonium tribromide (PTAB). Diazomethane and Zn-Cu, Diethyl maleate (DEM), Copper diacetylacetonate ($Cu(acac)_2$), $TiCl_3$, $NaIO_4$, Pyridinium chlorochromate (PCC), Pyridinium dichromate (PDC), Meisenheimer complex**.** Suzuki coupling, Heck reaction, Negishi reaction, Baylis-Hillman reaction.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. J. March and M. Smith, *Advanced Organic Chemistry*, 5th ed., John-Wiley and Sons. 2001. 2. E. S. Gould, *Mechanism and Structure in Organic Chemistry*, Holt, Rinehart and Winston Inc., 1959. 3. P. S. Kalsi, *Stereochemistry of carbon compounds*, 8thedn, New Age International Publishers, 2015. 4. P. Y.Bruice, *Organic Chemistry*, 7thedn.,Prentice Hall, 2013. 5. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee*Organic Chemistry*, 7th edn., Pearson Education, 2010.
Reference Books	1. S. H. Pine, *Organic Chemistry*, 5thedn, McGraw Hill International Editionn, 1987. 2. L. F. Fieser and M. Fieser, *Organic Chemistry*, Asia Publishing House, Bombay, 2000. 3. E.S. Gould, *Mechanism and Structure in Organic Chemistry*, Holt, Rinehart and Winston Inc., 1959. 4. T. L. Gilchrist, *Heterocyclic Chemistry*, Longman Press, 1989. 5. J. A. Joule and K. Mills, *Heterocyclic Chemistry*, 4thed., John-Wiley, 2010.
Website and e-learning	1.https://sites.google.com/site/chemistryebookscollection02/home/organic-chemistry/organic

source	2. https://www.organic-chemistry.org/

Course Learning Outcomes (for Mapping with POs and PSOs)
Students will be able:
CO1: To recall the basic principles of chemical reactions.
CO2: To understand the mechanism of various types of organic reactions.
CO3: To predict the suitable reagents for the conversion of selective organic compounds.
CO4: To correlate the principles of substitution, elimination, and addition reactions.
CO5: To design new routes to synthesis organic compounds.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="8">PHYSICAL CHEMISTRY-I</td></tr>
<tr><td>Paper No.</td><td colspan="8">Core VI – CC6</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td>Credits</td><td>4</td><td>Course Code</td><td colspan="2"></td></tr>
<tr><td>Semester</td><td>II</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="3">Total</td></tr>
<tr><td>4</td><td>1</td><td colspan="3">-</td><td colspan="3">5</td></tr>
<tr><td>Prerequisites</td><td colspan="8">Basic concepts of physical chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="8">To recall the fundamentals of thermodynamics and the composition of partial molar quantities.
To understand the classical and statistical approach of the functions.
To compare the significance of Maxwell-Boltzman, Fermi-Dirac and Bose-Einstein statistics.
To correlate the theories of reaction rates for the evaluation of thermodynamic parameters.
To study the mechanism and kinetics of fast reactions.</td></tr>
<tr><td rowspan="2">Course Outline</td><td colspan="8">UNIT-I: Classical Thermodynamics: Partial molar properties-Chemical potential, Gibb’s-Duhem equation-binary and ternary systems. Determination of partial molar quantities. Thermodynamics of real gases - Fugacity- determination of fugacity by graphical and equation of state methods-dependence of temperature, pressure and composition. Thermodynamics of ideal and non-ideal binary mixtures, Duhem - Margulus equation, applications of ideal and non-ideal mixtures. Activity and activity coefficients-standard states - determination-vapour pressure, EMF and freezing point methods.</td></tr>
<tr><td colspan="8">UNIT-II: Statistical thermodynamics: Introduction of statistical thermodynamics, concepts of thermodynamic and mathematical probabilities-distribution of distinguishable and non-distinguishable particles. Assemblies, ensembles, canonical particles. Maxwell - Boltzmann, Fermi Dirac & Bose-Einstein Statistics- comparison. Partition functions-evaluation of translational, vibrational and rotational partition functions for monoatomic, diatomic and polyatomic ideal gases. Thermodynamic functions in terms of partition functions-calculation of equilibrium constants. Statistical approach to Thermodynamic properties: pressure, internal energy, entropy, enthalpy, Gibb’s function, Helmholtz function, residual entropy and equilibrium constants. Heat capacity of mono and diatomic gases-ortho</td></tr>
</table>

	and para hydrogen. Heat capacity of solids-Einstein and Debye models.
	UNIT-III: Irreversible Thermodynamics: Theories of conservation of mass and energy, entropy production in open systems by heat, matter and current flow, force and flux concepts. Onsager theory-validity and verification- Onsager reciprocal relationships. Electro kinetic and thermo mechanical effects-Application of irreversible thermodynamics to biological systems.
	UNIT-IV: Kinetics of Reactions: Theories of reaction rates -effect of temperature on reaction rates, collision theory of reaction rates, Unimolecular reactions -Lindeman and Christiansen hypothesis. Potential energy surfaces. Transition state theory-evaluation of thermodynamic parameters of activation-applications of ARRT to reactions between atoms and molecules. Factors determine the reaction rates in solution - primary salt effect and secondary salt effect, Homogeneous catalysis- acid- base catalysis-mechanism of acid base catalyzed reactions-Bronsted catalysis law, enzyme catalysis-Michelis-Menton catalysis.
	UNIT-V: Kinetics of complex and fast reactions: Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions. Chain reactions-chain length, kinetics of H_2–Cl_2 & H_2–Br_2 reactions (Thermal and Photochemical reactions) - Rice Herzfeld mechanism. Study of fast reactions-relaxation methods-temperature and pressure jump methods, electric and magnetic field jump methods -stopped flow, flash photolysis methods and pulse radiolysis. Kinetics of polymerization-free radical, cationic, anionic polymerization - Polycondensation.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.

Recommended Text	1. J. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry, 2nd edition,S.L.N.Chand and Co., Jalandhar, 1986. 2. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th edition, W.A. BenjaminPublishers, California, 1972. 3. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt. Ltd., New Delhi, 1995. 4. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson, Reprint - 2013. 5. J. Rajaram and J.C. Kuriokose, Kinetics and Mechanisms of chemical transformation,M acmillan India Ltd, Reprint - 2011.
Reference Books	1. D.A. Mcqurrie And J.D. Simon, Physical Chemistry - A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999. 2. R.P. Rastogi and R.R. Misra, Classical Thermodynamics, Vikas Publishing, Pvt. Ltd., New Delhi, 1990. 3. S.H. Maron and J.B. Lando, Fundamentals of Physical Chemistry, Macmillan Publishers, New York, 1974 4. K.B. Ytsiimiriski, "Kinetic Methods of Analysis", Pergamom Press,1996. 5. Gurdeep Raj, Phase rule, Goel Publishing House, 2011.
Website and e-learning source	1. https://nptel.ac.in/courses/104/103/104103112/ 2. https://bit.ly/3tL3GdN

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To explain the classical and statistical concepts of thermodynamics.

CO2: To compare and correlate the thermodynamic concepts to study the kinetics of chemical reactions.

CO3: To discuss the various thermodynamic and kinetic determination.

CO4: To evaluate the thermodynamic methods for real gases ad mixtures.

CO5: To compare the theories of reactions rates and fast reactions.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">ORGANIC CHEMISTRY PRACTICAL - II</td></tr>
<tr><td>Paper No.</td><td colspan="7">Core VII – CC7</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td>Credits</td><td>3</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>II</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>-</td><td>1</td><td colspan="3">3</td><td colspan="2">4</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic concepts of organic chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the concept of quantitative estimation of organic compounds.
To develop analytical skill in the estimation of organic compounds.
To construct suitable experimental setup for the organic preparations involving two stages.
To experiment different purification and drying techniques for the compound processing.</td></tr>
<tr><td rowspan="2">Course Outline</td><td colspan="7">UNIT-I: Estimations:
a. Estimation of Phenol (bromination)
b. Estimation of Aniline (bromination)
c. Estimation of Ethyl methyl ketone (iodimetry)
d. Estimation of Glucose (redox)
e. Estimation of Ascorbic acid (iodimetry)
f. Estimation of Aromatic nitro groups (reduction)
g. Estimation of Glycine (acidimetry)
h. Estimation of Formalin (iodimetry)
i. Estimation of Acetyl group in ester (alkalimetry)</td></tr>
<tr><td colspan="7">UNIT-II: Two stage preparations:
a. p-Bromoaniline from acetanilide
b. p-Nitroaniline from acetanilide
c. 1,3,5-Tribromobenzene from aniline
d. Benzilic acid from benzoin
e. m-Nitroaniline from nitrobenzene
f. m-Nitrobenzoic acid from methyl benzoate</td></tr>
<tr><td>Extended Professional Component (is a part of internal component only, Not to be included in the external</td><td colspan="7">Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved
(To be discussed during the Tutorial hours)</td></tr>
</table>

examination question paper)	
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. A.I. Vogel, Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, 2011. 2. F.G. Mann and B.C. Saunders, Practical Organic Chemistry, 4th edn, Pearson Education India, 2009. 3. K. Bansal Raj, Laboratory Manual of Organic Chemistry, New Age International, 2009. 4. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, Basic Principles of Practical Chemistry, Sultan Chand & Sons, 2004. 5. V.K. Ahluwalia, and R. Aggarwal, Comprehensive Practical Organic Chemistry, Universities Press, 2004**.**
Reference Books	1. R.G. Engel, D.L. Pavia, G.M. Lampman and G.S. Kriz, *A Microscale approach to Organic Laboratory*, 5th edition, Paperback – International Edition, 2012. 2. P.B. Cranwell, L.M. Harwood and C.J. Moody, *Experimental Organic Chemistry*, 3rd edn, Wiley-Blackwell**,** 2017. 3. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, 3rd edn, CRC Press, 2013.
Website and e-learning source	https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistry-fall-2018/video_galleries/lecture-videos/
Course Learning Outcomes (for Mapping with POs and PSOs) Students will be able: **CO1**: To recall the basic principles of organic quantitative analysis. **CO2**: To explain the method of estimation of organic compounds. **CO3**: To develop the skills to estimate organic compounds. **CO4**: To develop the skills to handle corrosive and toxic chemicals in organic preparations. **CO5**:To categorize organic reactions and their mechanisms relevant to organic preparations.	

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	S	S	S	S	M	S	S	S	S	M
CO 2	M	S	S	S	S	M	S	S	S	S
CO 3	S	S	M	S	S	S	S	M	S	S
CO 4	M	S	S	S	S	M	S	S	S	S
CO 5	M	S	M	S	S	M	S	M	S	S

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to Pos	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">INORGANIC CHEMISTRY PRACTICAL-I</td></tr>
<tr><td>Paper No.</td><td colspan="7">Core VIII – CC8</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td>Credits</td><td>3</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>II</td><td colspan="4"></td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>-</td><td>1</td><td colspan="3">3</td><td colspan="2">4</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic principles of qualitative analysis</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To learn the principles and methods of qualitative analysis of familiar and less familiar cations present in a mixture.
To identify the methodology to analyze qualitatively a metal ion in the presence of another metal ion.
To recall the principle and theory in preparing standard solutions.
To train the students for improving their skill in estimating the amount of ion accurately present in the solution</td></tr>
<tr><td rowspan="2">Course Outline</td><td colspan="7">UNIT-I: Analysis of mixture of cations: Analysis of a mixture of four cations containing two common cations and two rare cations. Cations to be tested.
Group-I : W and Pb.
Group IA : Se, Te
Group-II : Mo, Cu, Bi and Cd.
Group-III : Ce, Th, Zr, V, Cr, and Ti.
Group-IV : Zn, Ni, Co and Mn.
Group-V : Ba and Sr.
Group-VI : Li.</td></tr>
<tr><td colspan="7">UNIT-II: Complexometric Titration:
1. Estimation of zinc, nickel, magnesium, and calcium.
2. Estimation of mixture of metal ions-pH control, masking and demasking agents.
3. Determination of calcium and lead in a mixture (pH control).
4. Determination of manganese in the presence of iron.
5. Determination of nickel in the presence of iron.</td></tr>
<tr><td>Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)</td><td colspan="7">Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved
(To be discussed during the Tutorial hours)</td></tr>
<tr><td>Skills acquired from this course</td><td colspan="7">Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.</td></tr>
<tr><td>Recommended Text</td><td colspan="7">1. A.JeyaRajendran, Microanalytical Techniques in Chemistry: Inorganic Qualitative Analysis, United global publishers, 2021.
2. V. V. Ramanujam, Inorganic Semimicro Qualitative Analysis; 3rded., The National Publishing Company, Chennai, 1974.</td></tr>
</table>

	3. Vogel's Text book of Inorganic Qualitative Analysis, 4thed., ELBS, London. 4. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, Vogel's Textbook of Quantitative Chemical Analysis, Revised 5th edition, ELBS, 1989. 5. Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, Fundamentals of Analytical Chemistry, 8th Edition, Brooks/Cole-Thomson Learning, USA, 2004.
Reference Books	1. G. Pass, and H. Sutcliffe, *Practical Inorganic Chemistry*; Chapman Hall, 1965. 2. W. G. Palmer, Experimental *Inorganic Chemistry*; Cambridge University Press, 1954.

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To explain the principles and techniques and have skills of qualitative analysis of familiar and less familiar cations in a mixture.

CO2: To analyze a metal ion in the presence of another metal ion.

CO3: To acquire the qualitative analytical skills by selecting suitable confirmatory tests and spot tests.

CO4: To describe the principles, techniques and skills related to quantitative determination of ions in a mixture by complexometric titration.

CO5: To estimate one metal ion in presence of another metal ion by complexometric method.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">MEDICINAL CHEMISTRY</td></tr>
<tr><td>Paper No.</td><td colspan="7">Elective III – EC3</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Elective</td><td>Year</td><td>I</td><td>Credits</td><td>3</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>II</td><td colspan="4"></td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>3</td><td>1</td><td colspan="3">-</td><td colspan="2">4</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of medicinal chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To introduce the mechanism of drug action and drug delivery system
To learn various types of drugs and their mode of action.
To learn drug design and drug synthesis.</td></tr>
<tr><td rowspan="5">Course Outline</td><td colspan="7">UNIT-I: Introduction to receptors: Introduction, targets, Agonist, antagonist, partial agonist. Receptors, Receptor types, Theories of Drug – receptor interaction, Drug synergism, Drug resistance, physicochemical factors influencing drug action.</td></tr>
<tr><td colspan="7">UNIT-II: Antibiotics: Introduction, Targets of antibiotics action, classification of antibiotics, enzyme-based mechanism of action, SAR of penicllins and tetracyclins, clinical application of penicillins, cephalosporin. Current trends in antibiotic therapy.</td></tr>
<tr><td colspan="7">UNIT-III: Antihypertensive agents and diuretics: Classification of cardiovascular agents, introduction to hypertension, etiology, types, classification of antihypertensive agents, Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol.
Classification and mechanism of action of diuretics, Furosemide, Hydrochlorothiazide, Amiloride.</td></tr>
<tr><td colspan="7">UNIT-IV: Antineoplastic Agents
Antineoplastic Agents: Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer - Introduction of carcinolytic antibiotics and mitotic inhibitors - Synthesis of mechlorethamine, cyclophosphamide, melphalan, and uracil - Recent development in cancer chemotherapy.</td></tr>
<tr><td colspan="7">UNIT-V: Analgesics, Anti-inflammatory and Antidiabetic Drugs: Introduction, Mechanism of inflammation, classification and mechanism of action and paracetamol, Ibuprofen, Diclofenac, naproxen, indomethacin, phenylbutazone and meperidine.</td></tr>
</table>

	Antidiabetic Agents: Introduction, Types of diabetics, Drugs used for the treatment, chemical classification, Mechanism of action, Treatment of diabetic mellitus. Chemistry of insulin, sulfonyl urea.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry, 2. Wilson, Charles Owens: Beale, John Marlowe; Block, John H, Lipincott William, 12th edition, 2011. 3. Graham L. Patrick, An Introduction to Medicinal Chemistry, 5th edition, Oxford University Press, 2013. Jayashree Ghosh, A text book of Pharmaceutical Chemistry, S. Chand and Co. Ltd, 1999, 1999 edn. 4. O. LeRoy, Natural and synthetic organic medicinal compounds, Ealemi, 1976. 5.S. Ashutosh Kar, Medicinal Chemistry, Wiley Eastern Limited, New Delhi, 1993, New edn.
Reference Books	1. Foye's Princles of Medicinal Chemistry, Lipincott Williams, Seventh Edition, 2012 2. Burger's Medicinal Chemistry, Drug Discovery and Development, Donald J. Abraham, David P. Rotella, Alfred Burger, Academic press, 2010. 3. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, John M. Beale Jr and John M. Block, Wolters Kluwer, 2011, 12th edn. 4. P. Parimoo, A Textbook of Medical Chemistry, New Delhi: CBS Publishers.1995. 5. S. Ramakrishnan, K. G. Prasannan and R. Rajan, Textbook of Medical Biochemistry, Hyderabad: Orient Longman. 3rd edition, 2001.
Website and e-learning source	1. https://www.ncbi.nlm.nih.gov/books/NBK482447/ 2. https://training.seer.cancer.gov/treatment/chemotherapy/types.html 3. https://www.classcentral.com/course/swayam-medicinal-chemistry-

	12908

Course Learning Outcomes (for Mapping with POs and PSOs)
Students will be able:
CO1: To predict drugs properties based on its structure.
CO2: To describe the factors that affect its absorption, distribution, metabolism, and excretion, and hence the considerations to be made in drug design.
CO3: To explain the relationship between drug's chemical structure and its therapeutic properties.
CO4: To give the knowledge of different theories of drug actions at molecular level.
CO5: To identify different targets for the development of new drugs for the treatment of cancer.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="8">GREEN CHEMISTRY</td></tr>
<tr><td>Paper No.</td><td colspan="8">Elective III – EC3</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Elective</td><td>Year</td><td>I</td><td>Credits</td><td>3</td><td>Course Code</td><td colspan="2"></td></tr>
<tr><td>Semester</td><td>II</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>3</td><td>1</td><td colspan="3">-</td><td colspan="2">4</td></tr>
<tr><td>Prerequisites</td><td colspan="8">Basic knowledge of general chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="8">To understand the basic principles of Green chemistry and Green techniques.
To study Green catalysis and Green solvents.
To propose solutions for pollution prevention in Industrial chemical and fuel production, Automotive industry and Shipping industries.
To propose green solutions for industrial production of Organic and inorganic chemicals.</td></tr>
<tr><td rowspan="4">Course Outline</td><td colspan="8">UNIT-I: Basic Principles of Green Chemistry: Introduction- Need for Green Chemistry. Goals of Green Chemistry. Limitations of Green Chemistry. Chemical accidents, terminologies, International green chemistry organizations and Twelve principles of Green Chemistry with examples.</td></tr>
<tr><td colspan="8">UNIT-II: Green Synthesis: Choice of starting materials, reagents, catalysts and solvents in detail, Green chemistry in day today life. Designing green synthesis-Green reagents: dimethyl carbonate. Green solvents: Water, Ionic liquids - criteria, general methods of preparation, effect on organic reaction. Supercritical carbon dioxide- properties, advantages, drawbacks and a few examples of organic reactions in $scCO_2$. Green synthesis-adipic acid and catechol.</td></tr>
<tr><td colspan="8">UNIT-III: Green Catalysis: Environmental pollution, Green Catalysis-Acid catalysts, Oxidation catalysts, Basic catalysts, Polymer supported catalysts-Poly styrene aluminum chloride, polymeric super acid catalysts, Polymer supported photosensitizers.</td></tr>
<tr><td colspan="8">UNIT-IV: Greener Reactions: Phase transfer catalysis in green synthesis-oxidation using hydrogen peroxide, crown ethers-esterification, saponification, anhydride formation, Elimination reaction, Displacement reaction. Applications in organic synthesis.</td></tr>
</table>

	UNIT-V: Green Techniques: Micro wave induced green synthesis - Introduction, Instrumentation, Principle and applications. Sonochemistry – Instrumentation, Cavitation theory - Ultra sound assisted green synthesis and Applications.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. Ahluwalia, V.K. and Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers, 2005. 2. W. L. McCabe, J.C. Smith and P. Harriott, Unit Operations of Chemical Engineering, 7th edition, McGraw-Hill, NewDelhi,2005. 3. J. M. Swan and D. St. C. Black, Organometallics in Organic Synthesis, Chapman Hall,1974. 4. V. K. Ahluwalia and R. Aggarwal, Organic Synthesis: Special Techniques, Narosa Publishing House, New Delhi,2001. 5. A. K. De, Environmental Chemistry, New Age Publications, 2017.
Reference Books	1. Anastas, P.T. and Warner, J.K. Oxford Green Chemistry -Theory and Practical, University Press, 1998 2. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker, 2001 3. Cann, M.C. and Connely, M.E. Real-World Cases in Green Chemistry, American Chemical Society, Washington, 2000 4. Ryan, M.A. and Tinnesand, M., Introduction to Green Chemistry, American Chemical Society Washington, 2002. 5. Chandrakanta Bandyopadhyay, An Insight into Green Chemistry, Books and Allied (P) Ltd, 2019.
Website and e-learning source	2. https://www.organic-chemistry.org/ 3. https://www.studyorgo.com/summary.php

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To recall the basic chemical techniques used in conventional industrial preparations and in green innovations.

CO2: To understand the various techniques used in chemical industries and in laboratory.

CO3: To compare the advantages of organic reactions assisted by renewable energy sources and non-renewable energy sources.

CO4: To apply the principles of PTC, ionic liquid, microwave and ultrasonic assisted organic synthesis.

CO5: To design and synthesize new organic compounds by green methods.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">BIO INORGANIC CHEMISTRY</td></tr>
<tr><td>Paper No.</td><td colspan="7">Elective IV – EC4</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Elective</td><td>Year</td><td>I</td><td>Credits</td><td>3</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>II</td><td colspan="4"></td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>3</td><td>1</td><td colspan="3">-</td><td colspan="2">4</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the role of trace elements.
To understand the biological significance of iron and sulphur.
To study the toxicity of metals in medicines.
To have knowledge on diagnostic agents.
To discuss on various metalloenzymes properties.</td></tr>
<tr><td rowspan="4">Course Outline</td><td colspan="7">UNIT-I: Essential trace elements: Selective transport and storage of metal ions: Ferritin, Transferrin and siderophores; Sodium and potassium transport, Calcium signaling proteins. Metalloenzymes: Zinc enzymes–carboxypeptidase and carbonic anhydrase. Iron enzymes–catalase, peroxidase. Copper enzymes – superoxide dismutase, Plast ocyanin, Ceruloplasmin, Tyrosinase. Coenzymes - Vitamin-B12 coenzymes.</td></tr>
<tr><td colspan="7">UNIT-II: Transport Proteins: Oxygen carriers - Hemoglobin and myoglobin - Structure and oxygenation Bohr Effect. Binding of CO, NO, CN^- to Myoglobin and Hemoglobin. Biological redox system: Cytochromes-Classification, cytochrome a, b and c. Cytochrome P-450. Non-heme oxygen carriers-Hemerythrin and hemocyanin. Iron-sulphur proteins- Rubredoxin and Ferredoxin- Structure and classification.</td></tr>
<tr><td colspan="7">UNIT-III: Nitrogen fixation: Introduction, types of nitrogen fixing microorganisms. Nitrogenase enzyme - Metal clusters in nitrogenase-Transition metal complexes of dinitrogen - nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia. Photosynthesis: photosystem-I and photosystem-II-chlorophylls structure and function.</td></tr>
<tr><td colspan="7">UNIT-IV: Metals in medicine: Metal Toxicity of Hg, Cd, Zn, Pb, As, Sb. Therapeutic Compounds: Vanadium-Based Diabetes Drugs; Platinum-Containing Anticancer Agents. Chelation therapy; Cancer treatment. Diagnostic Agents: Technetium Imaging Agents; Gadolinium MRI Imaging Agents.</td></tr>
</table>

	UNIT-V: Enzymes - Introduction and properties - nomenclature and classification. Enzyme kinetics, free energy of activation and the effects of catalysis. Michelis - Menton equation - Effect of pH, temperature on enzyme reactions. Factors contributing to the efficiency of enzyme.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. Williams,D.R. –Introdution to Bioinorganic chemistry. 2. F.M. Fiabre and D.R. Williams– The Principles of Bioinorganic Chemistry,RoyolSoceity of Chemistry, Monograph for Teachers-31 3. K.F. Purcell and Kotz., Inorganic chemistry, WB Saunders Co., USA. 4. G.N. Mugherjea and Arabinda Das, Elements of Bioinorganic Chemistry - 1993. 5. R. Gopalan, V. Ramalingam, *Concise Coordination Chemistry*, S. Chand, 2001.
Reference Books	1. M.Satake and Y.Mido, Bioinorganic Chemistry- Discovery Publishing House, New Delhi (1996) 2. M.N. Hughes, 1982, The Inorganic Chemistry of Biological processes, II Edition, Wiley London. 3. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987. 4. R. M. Roat-Malone, Bio Inorganic Chemistry, John Wiley, 2002. 5. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.
Website and e-learning source	1. https://www.pdfdrive.com/instant-notes-in-inorganic-chemistry-the-instant-notes-chemistry-series-d162097454.html 2. https://www.pdfdrive.com/shriver-and-atkins-inorganic-chemistry-5th-edition-d161563417.html
Course Learning Outcomes (for Mapping with POs and PSOs) Students will be able: **CO1**: To analyze trace elements. **CO2**: To explain the biological redox systems. **CO3**: To gain skill in analyzing the toxicity in metals. **CO4**: To get experience in diagnosis. **CO5**: To explain nitrogen fixation and photosynthetic mechanism.	

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">MATERIAL SCIENCE</td></tr>
<tr><td>Paper No.</td><td colspan="7">Elective IV – EC4</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Elective</td><td>Year</td><td>I</td><td>Credits</td><td>3</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>II</td><td colspan="4"></td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>3</td><td>1</td><td colspan="3">-</td><td colspan="2">4</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of solid-state chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the crystal structure, growth methods and X-ray scattering.
To explain the optical, dielectric and diffusion properties of crystals.
To recognize the basis of semiconductors, superconductivity materials and magnets.
To learn about the importance of materials used for renewable energy conversion.</td></tr>
<tr><td rowspan="3">Course Outline</td><td colspan="7">UNIT-I: Crystallography: symmetry - unit cell and Miller indices - crystal systems - Bravais lattices - point groups and space groups - X-ray diffraction-Laue equations-Bragg's law-reciprocal lattice and its application to geometrical crystallography. Crystal structure–powder and single crystal applications. Electron charge density maps, neutron diffraction-method and applications.</td></tr>
<tr><td colspan="7">UNIT-II: Crystal growth methods: Single crystal –Low and high temperature, solution growth– Gel and sol-gel. Crystal growth methods-nucleation– equilibrium stability and metastable state. Melt growth - Bridgeman-Stockbarger, Czochralski methods. Flux technique, physical and chemical vapour transport. Lorentz and polarization factor - primary and secondary extinctions.
Characterization–TG/DTA/DSC methods, SEM/TEM Analysis. Determination of Hardness, Applications of Single Crystals.</td></tr>
<tr><td colspan="7">UNIT-III: Properties of crystals: Optical studies - Electromagnetic spectrum (qualitative) refractive index – reflectance – transparency, translucency and opacity. Types of luminescence – photo-, electro-, and injection luminescence, LEDs – organic, Inorganic and polymer LED materials - Applications. Dielectric studies- Polarisation - electronic, ionic, orientation, and space charge polarisation. Effect of temperature. dielectric constant, dielectric loss. Types of dielectric breakdown–</td></tr>
</table>

	intrinsic, thermal, discharge, electrochemical and defect breakdown.
	UNIT-IV: Special Materials: Superconductivity: Meissner effect, Critical temperature and critical magnetic Field, Type I and II superconductors, BCS theory-Cooper pair, Applications. Soft and hard magnets – Domain theory Hysteresis Loop-Applications. Magneto and giant magnetoresistance. Ferro, ferri and antiferromagnetic materials-applications, magnetic parameters for recording applications. Ferro-, Piezo-, and pyro electric materials – properties and applications. Shape memory Alloys-characteristics and applications, Non-linear optics-Second Harmonic Generators, mixing of Laser wavelengths by quartz, ruby and $LiNbO_3$.
	UNIT-V: Materials for Renewable Energy Conversion: Solar Cells: Organic, bilayer, bulk heterojunction, polymer, perovskite based. Solar energy conversion: lamellar solids and thin films, dye-sensitized photo voltaic cells, coordination compounds anchored to semiconductor surfaces - Ru(II) and Os(II) polypyridyl complexes. Photochemical activation and splitting of water, CO_2 and N_2. Manganese based photo systems for water-splitting. Complexes of Rh, Ru, Pd and Pt - photochemical generation of hydrogen from alcohol.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. S. Mohan and V. Arjunan, Principles of Materials Science, MJP Publishers, 2016. 2. Arumugam, Materials Science, Anuradha Publications, 2007. 3. Giacavazzo et. al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010 4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012. 5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.
Reference Books	1.Suggested Readings 1. M.G. Arora, Solid State Chemistry, Anmol

	Publications, New Delhi, 2001. 2. R.K. Puri and V.K. Babbar, Solid State Physics, S Chand and Company Ltd, 2001. 3.. C. Kittel, Solid State Physics, John-Wiley and sons, NY, 1966. 4. H.P. Meyers, Introductory Solid State Physics, Viva Books Private Limited, 1998. 5. A.R. West, Solid State Chemistry and Applications, John-Wiley and sons, 1987.
Website and e-learning source	1. http://xrayweb.chem.ou.edu/notes/symmetry.html. 2. http://www.uptti.ac.in/classroom-content/data/unit%20cell.pdf. 3. https://bit.ly/3QyVg2R

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To understand and recall the synthesis and characteristics of crystal structures, semiconductors, magnets and renewable energy materials.

CO2: To integrate and assess the structure of different materials and their properties.

CO3: To analyse and identify new materials for energy applications.

CO4: To explain the importance of crystal structures, piezoelectric and pyroelectric materials, nanomaterials, hard and soft magnets, superconductors, solar cells, electrodes, LED uses, structures and synthesis.

CO5: To design and develop new materials with improved property for energy applications.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO 2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO 4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO 5	**M**	**S**	**M**	**S**	**S**	**M**	**S**	**M**	**S**	**S**

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

<table>
<tr><td>Title of the Course</td><td colspan="7">COMPUTATIONAL CHEMISTRY</td></tr>
<tr><td>Paper No.</td><td colspan="7">Skill Enhancement Course – SEC 1</td></tr>
<tr><td rowspan="2">Category</td><td rowspan="2">Core</td><td>Year</td><td>I</td><td>Credits</td><td>2</td><td>Course Code</td><td></td></tr>
<tr><td>Semester</td><td>II</td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="3">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>2</td><td>-</td><td colspan="3">2</td><td colspan="2">4</td></tr>
<tr><td>Prerequisites</td><td colspan="7">Basic knowledge of chemistry</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">To understand the concept of Computational chemistry.
To impart skills on use of various chemistry tools that are essential for any student with chemistry as a major course.
To learn the techniques of molecular simulations which will enhance the students' employability in academia and industry.</td></tr>
<tr><td rowspan="4">Course Outline</td><td colspan="7">UNIT- I: Basics: Need of Computational Chemistry – Tools of Computational Chemistry: Molecular Mechanics – Force field – Principles of Molecular mechanics – Merits and Demerits. Ab initio calculations: Principles of ab initio method – Hartree fock equations – Merits and Demerits. Semi empirical calculations : Basic principles – PPP, CNDO, INDO and NDDO methods – Merits and Demerits. Density Functional calculations – Basic principles – Kohn-Sham approach – Merits and Demerits.</td></tr>
<tr><td colspan="7">UNIT- II: Applications of Computational Chemistry: – Geometry optimization – Vibrational frequency analysis – Dipole moment – Bond order – Charges: Mulliken, Natural and Hirshfeld Charges – UV and NMR spectra, Electronegativity, Hardness, Softness, Fukui function.</td></tr>
<tr><td colspan="7">UNIT- III: Molecular Docking: Online servers for the selection of macromolecules and ligands – RCSB – Chemdata base – Online servers to detect druglikeness of compound - Swiss ADME – Molinspiration – ADMET servers – Preparation of macromolecule and ligand – Autodock Vina – Binding energy – Types of interactions between macromolecule and ligand - Molecular interaction visualizing softwares – Discovery Studio.</td></tr>
<tr><td colspan="7">UNIT- IV: Computing software – I: Introduction and stepwise approach to Chemdraw, ACD/Chemsketch and Argus Lab.
Exercises:
1. Drawing the structures of organic molecules and reaction schemes using Chemdraw or ACD/Chemsketch.</td></tr>
</table>

	2. Geometry optimization and single point energy calculations of simple organic molecules. 3. Calculation of dipole moment in polar organic molecules.
	UNIT- V: Computing Software – II: Introduction and stepwise approach to AVOGADRO, Molinspiration, SwissADME, SwissDock, and Autodock. **Exercises:** 1. Calculation of molecular properties and bioactivity of the simple drug molecules like aspirin, paracetamol, and the drugs of your choices using the online server molinspiration. 2. Prediction of drug likeliness, ADME and Toxicity of the drug classes like antibiotics, antihistamines, anesthetics and drug molecules of your choice using online server SwissADME or SwissDock. 3. Perform molecular docking of your choice using Autodock tools or Autodock Vina or Argus Lab.
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.
Recommended Text	1. Frank Jensen, Introduction to Computational Chemistry, Third Edition, John Wiley & Sons, 2017. 2. Andrew R. Leach, Molecular modelling: principles and applications, Second Edition, Prentice-Hall, 2001. 3. Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, Second Edition, John Wiley & Sons, 2004.
Reference Books	1. Jan H. Jensen, Molecular Modelling Basics, CRC Press, 2010. 2. Waren J. Hehre, Alan J. Shusterman and Janet E. Nelson, The molecular modelling workbook for organic chemistry, Wavefunction Inc., 1998. 3. James B. Foresman and Eleen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., Third Edition, 2015.

Website and e-learning source	1. https://onlinecourses.nptel.ac.in/noc20_cy08/preview 2. https://www.digimat.in/nptel/courses/video/104106122/L14.html

Course Learning Outcomes (for Mapping with POs and PSOs)

Students will be able:

CO1: To describe the basic and need of Computational Chemistry.

CO2: To understand the applications of Computational Chemistry methods.

CO3: To gain knowledge about the Molecular docking.

CO4: To use chemical software for drawing chemical structures, reaction schemes and generation of their names.

CO5: To perform molecular docking in structural molecular biology and computer assisted drug design which enhance their employability in academia and industry.

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	S	S	S	S	M	S	S	S	S	M
CO 2	M	S	S	S	S	M	S	S	S	S
CO 3	S	S	M	S	S	S	S	M	S	S
CO 4	M	S	S	S	S	M	S	S	S	S
CO 5	M	S	M	S	S	M	S	M	S	S

3 – Strong, 2 – Medium, 1 - Low

Level of Correlation between PSO's and CO's

CO /PSO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to PSOs	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low