PG AND RESEARCH DEPARTMENT OF CHEMISTRY

POOMPUHAR COLLEGE (AUTONOMOUS)

MELAIYUR, 609107.

(Affiliated to Annamalai University)

M.Sc. Chemistry

CHOICE BASED CREDIT SYSTEM
SYLLABUS
2023 – 2024 ONWARDS

PG AND RESEARCH DEPARTMENT OF CHEMISTRY
POOMPUHAR COLLEGE (AUTONOMOUS)
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Programme Structure and Scheme of Examination (under CBCS)
(Applicable to the candidates admitted from the academic year 2023 -2024 onwards)

Part	Study Components & Course Title	Credit	Hours/ Week	Maximum Marks		
				CIA	ESE	Total
	SEMESTER – I					
Part A	Core - I: Organic Reaction Mechanism-I	5	7	25	75	100
	Core - II: Structure and Bonding in Inorganic Compounds and Nuclear Chemistry	5	7	25	75	100
	Core - III: Organic Chemistry Practical	4	6	25	75	100
	Elective – I (Discipline centric) Pharmaceutical Chemistry Nanomaterials and Nanotechnology	3	5	25	75	100
	Elective-II (Generic centric) Electrochemistry Molecular Spectroscopy	3	5	25	75	100
	Total	**20**	**30**			**500**
	SEMESTER – II					
Part A	Core - IV: Organic Reaction Mechanism–II	5	6	25	75	100
	Core - V: Physical Chemistry–I	5	6	25	75	100
	Core - VI: Inorganic Chemistry Practical	4	6	25	75	100
	Elective – III (Discipline centric) Medicinal Chemistry Green Chemistry	3	4	25	75	100
	Elective – IV (Generic centric) Bio Inorganic Chemistry Material Science	3	4	25	75	100
Part B	Skill Enhancement Course (SEC-I): Industrial Chemistry and Computational Software in Chemistry	2	4	25	75	100
	Total	**22**	**30**			**600**

Core-I	ORGANIC REACTION MECHANISM - I	Credit	5
I Year		Hours/ Week	7
I Semester			

Objectives of the course	• 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.
Course Outline	**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: non-kinetic methods - product analysis, determination of intermediates-isolation, detection, and trapping. Cross-over experiments, isotopic labelling, isotope effects and stereo chemical evidences. Kinetic methods - relation of rate and mechanism.Effect of structure on reactivity: Hammett and Taft equations. Linear free energy relationship, substituent and reaction constants.
	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; 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 attackingnucleophile. Reactions: Oxygen and Sulphur-nucleophiles, Bucherer and Rosenmund reactions, von Richter, Sommelet- Hauser and Smiles rearrangements. 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. Topicityand prostereoisomerism,prochirality, enantiotopic and diastereotopic atoms, groups, faces, axial and planar chirality, chirality due to helical shape. Cram's and Prelog's rules. Configurations of allenes, spiranes, biphenyls, cyclooctene, Cycloalkanes. shift reagents and chiral solvating reagents. Optical purity, criteria for optical purity: Resolution of racemic modifications, asymmetric synthesis. 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 poly substituted 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. 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 Learning Outcomes (for Mapping with POs and PSOs)

Students will be able

CLO1: To recall the basic principles of organic chemistry.

CLO2: To understand the formation and detection of reaction intermediates of organic reactions.

CLO3: To predict the reaction mechanism of organic reactions and stereochemistry of organic compounds.

CLO4: To apply the principles of kinetic and non-kinetic methods to determine the mechanism of reactions.

CLO5:To design and synthesize new organic compounds by correlating the

stereochemistryof 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 /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

Core-II	23AU:P01M2	Credit	5
I Year	STRUCTURE AND BONDING IN INORGANIC COMPOUNDS AND NUCLEAR CHEMISTRY	Hours/Week	7
I Semester			

Objectives of the course	• To determine the structural properties of main group compounds and clusters. • To gain fundamental knowledge on the structural aspects of ionic crystals. • To familiarize various diffraction and microscopic techniques. • To study the effect of point defects and line defects in ionic crystals. • To evaluate the structural aspects of solids. • To study about stellar energy, nuclear reactions etc and to equip the students for their future career in nuclear industry.
Course Outline	**UNIT-I: Structure of main group compounds and clusters:** VB theory: Structure of silicates - applications of Paulings 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 structure of borane cluster; main group clusters –zintl ions and mno rule.
	UNIT-II: Solid state chemistry: Ionic crystals: Packing of ions in simple, hexagonal and cubic close packing, voids in crystal lattice, Radius ratio, Crystal systems and Bravis lattices, Solid state energetics: Lattice energy – Born-Lande equation - Kapustinski equation, Madelung constant. 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.
	UNIT-III: Techniques in solid state chemistry: X-ray diffraction technique: Bragg's law, Powder diffraction method – Principle and Instrumentation; Interpretation of XRD data – JCPDS files, Phase purity, Scherrer formula, lattice constants calculation; Systematic absence of reflections; Electron diffraction technique – principle, instrumentation and application. Electron microscopy – difference between optical and electron microscopy, theory, principle, instrumentation, sampling methods and applications of SEM and TEM.
	UNIT-IV: 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, laser and phosphors; Linear defects and its effects due to dislocations.
	UNIT– V:Nuclear Chemistry

	Nuclear properties: Nuclear spin and moments, origin of nuclear forces, **Modes of radioactive decay:** Orbital electron capture, nuclear isomerism, internal conversion. **Nuclear reactions:** Types, cross section, compound nucles theory, high energy nuclear, direct nuclear, photonuclear and thermonuclear reactions. **Stellar energy:** synthesis of elements, hydrogen burning, carbon burning **Particle accelerators:** Linear accelerators, cyclotron and synchrotron. **Radio analytical methods:** Isotope dilution analysis, radiometric titrations, Neutron activation analysis.
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. 6. Arnikar, H. J. (2005). *Essentials of nuclear chemistry*. New Age International (P) Ltd. 7. Frielander, G., Kennedy, J. W., & Miller, J. M. (1981). *Nuclear and Radiochemistry*.John Wiley and Sons.
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: Predict the geometry of main group compounds and clusters.
CO2: Explain about the packing of ions in crystals and apply the radius ratio rule to predict the coordination number of cations.
CO3: Understand the various types of ionic crystal systems and analyze their structural features.
CO4: Explain the crystal growth methods.
CO5:To understand the principles of diffraction techniques and microscopic 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 Pos	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 - Low

Core-III	ORGANIC CHEMISTRY PRACTICAL	Credit	4
I Year		Hours/Week	6
I Semester			

Objectives of the course	• To understand the concept of separation, qualitative analysis and preparation of organiccompounds. • To develop analytical skill in the handling of chemical reagents for separation of binary and ternaryorganic mixtures. • To analyze the separated organic components systematically and derivative them suitably. • To construct suitable experimental setup for the organic preparations involving two stages. • To experiment different purification and drying techniques for the compound processing.
Course Outline	**UNIT-I: Separation and analysis:** Two component mixtures
	UNIT-II: **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) j) Estimation of Hydroxyl group (acetylation) **k)** Estimation of Amino group (acetylation)
	UNIT-III: Two stage preparations: a) *p*-Bromoacetanilide from aniline b) *p*-Nitroaniline from acetanilide c) 1,3,5-Tribromobenzene from aniline d) Acetyl salicyclic acid from methyl salicylate e) Benzilic acid from benzoin f) *m*-Nitroaniline from nitrobenzene g) *m*-Nitrobenzoic acid from methyl benzoate
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. N.S.Gnanaprakasam andG.Ramamurthy, Organic Chemistry Lab Manual, S.V.Printers, 2007. 2. Raj.K.Bansal, Laboratory Manual of Organic Chemistry, New Age International Publishers, 4th edition, 2001. 3. A.I.Vogel, A.R.Tatchell, B.S.Furniss, A.J.Hannaford and P.W.G.SmithVogel's Textbook of Practical Organic Chemistry,

	Prentice Hall, 5th edition, 1989.
Reference Books	1.F.G. Mann and B.C. Saunders, *Practical Organic Chemistry*, 4th edn, Pearson Education India, 2009. 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 Organic Chemistry*, Universities Press, 2004**.** 5. 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. 6. P.B. Cranwell, L.M. Harwood and C.J. Moody, *Experimental Organic Chemistry*, 3rd edn, Wiley-Blackwell**,** 2017. 7. J. Leonard, B. Lygo and G. Procter, *Advanced Practical Organic Chemistry*, 3rd edn, CRC Press, 2013. 8. Moore, Dalrympk and Rodig, *Experimental methods in organic chemistry*, 3rd edition, Saunders College publishing, The Oxford Press, 1982.
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 separation, qualitative analysis and preparation.

CO2: To explain the method of separation and analysis of separated organic mixtures and convert them as derivatives by suitable preparation method.

CO3: To determine the characteristics of separation of organic compounds by various chemical reactions.

CO4: To develop strategies to separate, analyze and prepare organic compounds.

CO5:To formulate a method of separation, analysis of organic mixtures and design suitable procedure for 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

Elective I	23AU:P01E1	Credit	3
I Year	NANO MATERIALS AND NANO TECHNOLOGY	Hours Week	5
I Semester			

Objectives of the course	• 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.
Course Outline	**UNIT-I:** Introduction of nanomaterials and nanotechnologies, Introduction-role of size, classification-0D, 1D, 2D, 3D. Synthesis-Bottom –Up, Top–Down, consolidation of Nano powders.Features of nanostructures, Background of nanostructures.Techniques of synthesis of nanomaterials, Tools of the nanoscience. Applications of nanomaterials and technologies.
	UNIT-II: 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.
	UNIT-III: Mechanical properties of materials, theories relevant to mechanical properties.Techniques to study mechanical properties of nanomaterials, adhesion and friction, thermal properties of nanomaterialsNanoparticles: gold and silver, metal oxides: silica, iron oxide andalumina - synthesisandproperties.
	UNIT-IV: Electrical properties, Conductivity and Resistivity, Classification of Materials 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 thin films, nanocomposites. Application of nanoparticles in different fields. Core-shellnanoparticles-types,synthesis,andproperties.Nanocomposites-metal-,ceramic-andpolymer-matrixcomposites-applications. Characterization– SEM, TEM and AFM - principle,instrumentationand 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. C. N. R. Rao, A. Muller and A. K. Cheetham (Eds), The Chemistry of Nanomaterials: Vol. 1 and 2; Wiley-VCH;Germany, Weinheim, 2004. 2. C. P. Poole, Jr: and F. J. Owens, Introduction to Nanotechnology; Wiley Interscience, New Jersey, 2003. 3. K. J. Klabunde (Ed), Nanoscale Materials in Chemistry; 2nd Ed., Wiley- Interscience, New York, 2009. 4. T. Pradeep, Nano: The Essentials in Understanding Nanoscience and Nanotechnology; 1st Ed., Tata McGraw Hill, New York, 2007. 5. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties, Elsevier, Chennai, 2000 6.Rajendra Kumar Goyal, *Nanomaterials and Nanocomposites: Synthesis, Properties, Characterization Techniques, and Applications***,** First edition, CRC Press, 2018. 7. Joseph Koo, *Polymer Nanocomposites*, First Edition, McGraw-Hill, 2006. 8. Sati N. Bhattacharya, Musa R. Kamal and Rahul K. Gupta, *Polymeric Nanocomposites - Theory and Practice* Hanser Gardner Publications, 2.008. 9.Guozhong, *Nanostructures and Nanomaterials: Synthesis, Properties and Applications,* Imperial College Press, 2004. 10. Edited by Vikas Mittal, *Synthesis Techniques for Polymer Nanocomposites*, Wiley-VCH, 2015.
Reference Books	1.AhmetGürses, *Introduction to Polymer–Clay Nanocomposites*, CRC Press, 2016. 2. T. Tang and P. Sheng (Eds), Nanoscience and Technology, Novel Structures and Phenomena; Taylor andFrancis, New York, 2003. 3. R. Booker, E. Boysen, Nanotechnology - The fun and easy way to explore the science of matter's smallest particles; Wiley – dreamtech, Newdelhi, Reprint 2007.
Website and e-learning source	1. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/ 2. Nanoletters - http://pubs.acs.org/journals/nalefd/index.html 3. Nanotation- http://www.acsnanotation.org/

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
CO1	S	S	S	S	M	S	S	S	S	M
CO2	M	S	S	S	S	M	S	S	S	S
CO3	S	S	M	S	S	S	S	M	S	S
CO4	M	S	S	S	S	M	S	S	S	S
CO5	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

Elective II	MOLECULAR SPECTROSCOPY	Credit	3
I Year		Hours/ Week	5
I Semester			

Objectives of the course	• To understand the influence of rotation and vibrations on the spectra of the polyatomic molecules. • To study the principle of Raman spectroscopy, ESR spectroscopy, EPR 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.
Course Outline	**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-O and S branches.
	UNIT-II: Vibrational Spectroscopy: Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, 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 on vibrational spectra of polyatomic molecule.
	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 ESR spectroscopy: 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 type. Vicinal, geminal and long-range coupling-spin decoupling. Nuclear Overhauser effect (NOE). ^{13}CNMRand structural correlations, Satellites. Brief introduction to 2D NMR – COSY, NOESY. Introduction to ^{31}P, ^{19}F NMR. ESR spectroscopy Characteristic features of ESR spectra, line shapes and line widths; 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;

	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.
	UNIT-V: Mass Spectrometry, EPR and Mossbauer Spectroscopy: 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.EPR spectra of anisotropic systems - anisotropy in g-value, anisotropy in hyperfine coupling, hyperfine splitting caused by quadrupole nuclei. Principle of Mossbauer spectroscopy: Doppler shift, recoil energy. Isomer shift, quadrupole splitting, magnetic interactions. Applications: Mossbauer spectra of high and low-spin Fe compounds. Structural elucidation of organic compounds by combined spectral techniques.
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. 6. Sharma, Y. R. Structural identification of organic compounds. S. Chand & Co.
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}FNMR.

CO5:To develop the knowledge on principle, instrumentation and structural elucidation ofsimple molecules using Mass Spectrometry.

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

Core –IV	ORGANIC REACTION MECHANISM-II	Credit	5
I Year		Hours/ Week	6
II Semester			

Objectives of the course	• To understand the concept of aromaticity in benzenoid, non-benzenoid, heterocyclic and annulene compounds. • To understand the mechanism involved in various types of organic reactions with evidences. • To understand the applications of synthetically important reagents. • To correlate the reactivity between aliphatic and aromatic compounds. • To design synthetic routes for synthetically used organic reactions.
Course Outline	**UNIT-I: Elimination and Free Radical Reactions:** Mechanisms: E2, E1, and E1cB mechanisms. Syn- and anti-eliminations. 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 radical reactions and free radical, reactions of radicals; polymerization, addition, halogenations, aromatic substitutions, rearrangements. Reactivity: Reactivity on aliphatic, aromatic substrates, reactivity in the attacking radical, effect of solvent.
	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, osmium tetroxide, oxidation of saturated hydrocarbons, alkyl groups, alcohols, halides and amines. 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 dimethyl sulphoxide- dicyclohexylcarbodiimide (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, Dienone-phenol, Baker-Venkataraman, 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, Cope, oxy-Cope Benzidine rearrangements.
	UNIT-IV: Addition to Carbon Multiple Bonds: Mechanisms: (a) 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; (b) Addition to carbon-

	hetero atom multiple bonds: Mannich reaction, acids, esters, nitrites, addition of Grignard reagents, Wittig reaction, Prinsreaction. Addition to Carbon-Hetero atom Multiplebonds: Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. 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), Azobisisobutyronitrile (AIBN), Sodium cyanoborohydride ($NaBH_3CN$), *meta*-Chloroperbenzoic acid (m-CPBA), Dimethyl aminiopyridine (DMAP), Diisopropylazodicarboxylate (DIAD), Diethylazodicarboxylate (DEAD), *N*-bromosuccinimide (NBS), Tetramethyl piperiridin-1-oxyl (TEMPO), Phenyltrimethylammoniumtribromide (PTAB).Diazomethane and Zn-Cu, Diethyl maleate (DEM), Pyridinium chlorochromate (PCC),Pyridinium dichromate (PDC), Meisenheimer complex**.** Suzuki coupling, Heck 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. BhattacharjeeOrganic 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. Carruther, Jain Coldham, Modern Methods of organic synthesis, IV Edition. 5. W.Carruthers,Some Modern Methods of Organic Synthesis,IIIEdition,Cambridge University Press, (1993). Wiley, 2010.
Website and e-learning source	1.https://sites.google.com/site/chemistryebookscollection02/home/organic-chemistry/organic 2. https://www.organic-chemistry.org/
Course Learning Outcomes (for Mapping with POs and PSOs)	

Students will be able:
CO1: To recall the various mechanisms of rearrangements
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 /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

Core – V	PHYSICAL CHEMISTRY-I	Credit	5
I Year		Hours/ Week	6
II Semester			

Objectives of the course	• 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 • To correlate the theories of reaction rates for the evaluation of thermodynamic parameters. • To study the mechanism and kinetics of reactions.
Course Outline	**UNIT-I: Classical Thermodynamics:** Partial molar properties-Chemical potential, Gibb's-Duhem equation-binary and ternary systems. Determination of partial molar quantities. Fugacity-determination of fugacity bygraphical 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-EMF method.
	UNIT-II: Statistical thermodynamics: Introduction of statistical thermodynamicsconcepts of thermodynamic and mathematicalprobabilities-distribution of distinguishable and non-distinguishable particles.Assemblies, ensembles, canonical particles. Maxwell - Boltzmann, Fermi Dirac & Bose-Einstein Statistics-comparison and applications.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, equilibrium constants and equipartition principle. 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 reactions-effect of temperature on reaction rates, collision theory of reaction rates, Unimolecular reactions -Lindeman and Christiansen hypothesis-molecular beams,collision cross sections, effectiveness of collisions,Potential energy surfaces. Transition state theory-evaluation of thermodynamicparameters of activation-applications of ARRT to reactions between atoms and molecules, Kinetic parameter evaluation. 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, reversiblereactions, 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) - Study of fast reactions- temperature and pressure jump methods - stopped flow flash photolysis methods. 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,Macmillan 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 /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

Core – VI	INORGANIC CHEMISTRY PRACTICAL	Credit	4
I Year		Hours/ Week	6
II Semester			

Objectives of the course	• To understand and enhance the visual observation as an analytical tool for the quantitative estimation of ions. • 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 • To estimate metal ions, present in the given solution accurately without using instruments. • To determinethe amount of ions, present in a binary mixture accurately.
Course Outline	**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, Tl and Pb. Group-II : Se, Te, Mo, Cu, Bi and Cd. Group-III : Tl, Ce, Th, Zr, V, Cr, Fe, Ti and U. Group-IV : Zn, Ni, Co and Mn. Group-V : Ca, Ba and Sr. Group-VI : Li and Mg.
	UNIT-II: Preparation of metal complexes: Preparation of inorganic complexes: a. Preparation of tristhioureacopper(I)sulphate b. Preparation of potassium trioxalate chromate(III) c. Preparation of tetramminecopper(II) sulphate d. Preparation of Reineck's salt e. Preparation of hexathioureacopper(I) chloridedihydrate f. Preparation of *cis*-Potassium tri oxalate diaquachromate(III) g. Preparation of sodium trioxalatoferrate(III) h. Preparation of hexathiourealead(II) nitrate
	UNIT-III: 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.
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. 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. 3. *Vogel's Text book of Inorganic Qualitative Analysis,* 4thed., ELBS, London. **Reference Books :**
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. 3.Basic principles of practical chemistry, V. Venkateswaran, R. Veeraswamy and A.R. Kulandaivelu, Sultan Chand & Sons, 2nd edition, 1997.
Course Learning Outcomes (for Mapping with POs and PSOs) Students will be able: **CO1**: To identify the anions and cations present in a mixture of salts. **CO2**: To apply the principles of semi micro qualitative analysis to categorize acid radicals and basic radicals. **CO3**: To acquire the qualitative analytical skills by selecting suitable confirmatory tests andspot tests. **CO4**: To choose the appropriate chemical reagents for the detection of anions and cations. **CO5**:To synthesize coordination compounds in good quality.	

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

Elective III	**GREEN CHEMISTRY**	**Credit**	**3**
I Year		**Hours /Week**	**4**
II Semester			

Objectives of the course	• To discuss the principles of green chemistry, • To propose green solutions for chemical energy storage and conversion. • To propose green solutions for industrial production of Petroleum and Petrochemicals. • 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 Surfactants, Organic and inorganic chemicals.
Course Outline	**UNIT-I:** 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.
	UNIT-II: 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.
	UNIT-III: Environmental pollution, Green Catalysis-Acid catalysts, Oxidation catalysts, Basic catalysts, Polymer supported catalysts-Poly styrene aluminum chloride, polymeric super acid catalysts, Poly supported photosensitizers.
	UNIT-IV: Phase transfer catalysis in green synthesis-oxidation using hydrogen peroxide, crown ethers-esterification, saponification, anhydride formation, Elimination reaction, Displacement reaction. Applications in organic synthesis.
	UNIT-V: 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	1. Ahluwalia, V.K. and Kidwai, M.R. New Trends in Green Chemistry,

Text	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. ChandrakantaBandyopadhyay, An Insight into Green Chemistry, Books and Allied (P) Ltd, 2019.
Website and e-learning source	1. https://www.organic-chemistry.org/ 2. 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 /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

Elective IV	BIO-INORGANIC CHEMISTRY	Credit	3
I Year		Hours/ Week	4
II Semester			

Objectives of the course	• To understand the role of trace elements. • To understand the biological significance of iron, sulpur. • To study the toxicity of metals in medicines. • To have knowledge on diagnostic agents. • To discuss on various metalloenzymes properties.
Course Outline	**UNIT-I: Essential trace elements:** Selective transport and storage of metal ions: Ferritin, Transferrin and sidorphores; Sodium and potassium transport, Calcium signalling proteins.Metallo enzymes: Zinc enzymes–carboxypeptidase and carbonic anhydrase. Ironenzymes–catalase, peroxidase. Copperenzymes – superoxide dismutase, Plastocyanin, Ceruloplasmin, Tyrosinase.
	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.
	UNIT-III: Nitrogen fixation-Introduction, types of nitrogen fixing microorganisms. Nitrogenase enzyme - Metal clusters in nitrogenase-redox property - Dinitrogen complexes transition metal complexes of dinitrogen - nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia.
	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.
	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**. 6. K. Hussain Reddy , Bioinorganic Chemistry.
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 Biologicalprocesses, 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: The students will be able to analyses trace elements.

CO2: Students will be able to explain the biological redox systems.

CO3: Students will gain skill in analyzing the toxicity in metals.

CO4: Students will have experience in diagnosis.

CO5: Learn about the 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 /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

PART-B	INDUSTRIAL CHEMISTRY AND COMPUTATIONAL SOFTWARE IN CHEMISTRY	Credit	2
I Year		Hours/ Week	4
II Semester			

Objectives of the course	To gain knowledge about industrial fuels. To understand the importance of leather and water industry. To study about small scale industries. 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.
Course Outline	**UNIT-I: Industrial fuels** Fuels and Energy Resources: Types of fuels - liquid fuels - petroleum products – gaseous fuel - coal gas, producer gas and biogas - Rocket fuels - solid and liquid propellants - nuclear fuels - difference between nuclear and chemical fuels. Renewable sources of energy - solar energy, wind energy and tidal energy.
	UNIT-II: Leather Industry and Water Industry Leather Industry: Curing-preservation and tanning of hides and skins-Process of dehairing and dyeing - Treatment of tannery effluents. Water Industry: Pollution of water by fertilizers, pesticides and industrial wastes -BOD-COD-thermal pollution. Reverse osmosis- softening of hard water.
	UNIT-III: Small Scale Chemical Industries Electro thermal and electrochemical industries: electroplating - surface coating industries - oils, fats and waxes. Match industries and fireworks manufacture of some industrially important chemicals like potassium chlorate- and red phosphorus. .
	UNIT-IV: **- BASICS** Basic idea of Molecular Modelling – A brief introduction about computational methods and their applications in chemistry – Basic terminologies used in computational methods Software – List of software used in computational chemistry- Introduction and stepwise approach to Chem draw, Argus lab, Gaussian, Gauss view, Autodoc and Schrödinger software
	UNIT-V: **HANDS ON EXERCISES** Principles of Docking: Docking Protein-protein docking. Glide score Combiglide - Receptor grid generation, reagent preparation, combinatorial screening, combinatorial library enumeration, interactive enumeration and docking. Desmondsystem builder, minimization, molecular dynamics, Hands on Training (Not for examination) The experiments are related to the topics covered in B.Sc - M.Sc Chemistry courses. The students must do the following exercises depending on the availability of time and suitable computational chemistry software.

	Drawing the structures of organic molecules and reaction schemes using **Chemdraw** or **ACD/Chem sketch**. **B.** For the following experiments, **Argus Lab** or **ACD/Chemsketch** or **Avogadro Molecular Editor** or **Gaussian software** can be used. Minimum of six experiments are required to be carried out in this section. 1. Geometry optimization and single point energy calculations of simple organic molecules. 2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals. 3. Calculation of dipole moment in polar organic molecules. 4. Calculation of electrostatic charges of atoms in organic molecules using population analysis. 5. Calculation of Resonance energy of aromatic compounds. Prediction of the stability of *ortho*, *meta*, *para* products of nitration of aromatic ring using computational chemistry calculations. 7. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules. 8. Calculation of dimerization energy of carboxylic acids. 9. Perform the conformational analysis of butane using potential energy scan. 10. Find the transition state of simple organic reactions and plot the reaction profile. **C.** Prediction of molecular properties, bioactivity and molecular docking of drug molecules. 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 servers **preADMET**or **SwissADME**or **SwissDock.**
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. Biswas, A. K. (1989). *Frontiers in Applied Chemistry*. Narosa publishing house. 2. Vermain, O. P & Narula, A. C. (2014). A*pplied chemistry theory and books.* National Publishers.

Reference Books	1. Shreve, R. N., & Brink, J. A. (1977). *Chemical Process Industries* (4th edn.). Tokyo: McGraw Hill. 2. Chakrabarty, N. (1981). *Industrial Chemistry.* New Delhi: Oxford& Publishing Co. 3. Singh, P. P., Joseph, T. M., &Dhavale, R. G. (1983). *College Industrial Chemistry* (4th edn.).Bombay: Himalaya Publishing House. 4. Jan H. Jensen, *Molecular Modelling Basics*, CRC Press, 2010. 5. Waren J. Hehre, Alan J. Shusterman and Janet E. Nelson, *The molecular modelling workbook for organic chemistry*, Wavefunction Inc., 1998. 6. James B. Foresman and Eleen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., Second Edition, 1996. 7. James B. Foresman and Eleen Frisch, *Exploring Chemistry with Electronic Structure Methods,* Gaussian Inc., Third Edition, 2015. 8. Donald W. Rogers, H*eats of Hydrogenation: Experimental and Computational Hydrogen Thermochemistry of Organic compounds*, World scientific Publishing Co, 2006.
Website and e-learning source	1. http://ecoursesonline.iasri.res.in>mod>page 2. https://www.neratanning.com>leathertanning 3. https://en.wikipedia.org>wiki>Electroplating 4. https://www.civilgiant.com>manufacture-of-cement 5. https://www.researchgate.net>...>Molasses **LINKS TO DOWNLOAD SOFTWARE** ACD/Chemsketch : https://www.acdlabs.com/resources/freeware/chemsketch/index.php Molinspiration : https://www.molinspiration.com/ PreADMET : https://preadmet.bmdrc.kr/ SwissADME : http://www.swissadme.ch/index.php Crystal Explorer: https://crystalexplorer.scb.uwa.edu.au/ 1-click docking online server: https://mcule.com/ Autodock Tools Link: http://mgltools.scripps.edu/downloads AutodockVina Link: http://vina.scripps.edu/ Discovery Studio Visualizer: https://www.3dsbiovia.com/products/co.. Avogadro Molecular Editor : https://avogadro.cc/ ArgusLab : http://www.arguslab.com/arguslab.com/ArgusLab.html **Course Learning Outcomes (for Mapping with POs and PSOs)** Students will be able: **CO1**: Students will be able to acquire knowledge of industrial fuels. **CO2**: Illustrate the importance of leather and water industries. **CO3**: Acquire knowledge about small scale industries. **CO4**: Acquire knowledge about chemistry software's . CO5: Acquire knowledge about techniques of molecular simulations

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**
CO2	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO3	**S**	**S**	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**
CO4	**M**	**S**	**S**	**S**	**S**	**M**	**S**	**S**	**S**	**S**
CO5	**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

SCHEME OF VALUATION FOR ORGANIC PRACTICALS

Semester Examination	Marks (75)
Analysis	30
Estimation	20
preparation	10
Viva - voce	10
Record	05
Total	75

INTERNAL ASSESSMENT	Marks
Attendance / Regularity	**10**
Results /accuracy	**15**
Total	**25**

SCHEME OF VALUATION FOR INORGANIC PRACTICALS

Semester Examination	Marks (75)
Analysis of mixture	30
Complexometric titration	20
Preoaration	10
Viva - voce	10
Record	05
Total	75

INTERNAL ASSESSMENT	Marks
Attendance / Regularity	**10**
Results /accuracy	**15**
Total	**25**