M. Sc., Chemistry Syllabus for year 2020-21

Programme Outcomes (PO)

PO1: Demonstrate the advanced theories, theorems and coherent understanding variety of field ofscience, its different branches, diversified thinking and its linkage with other disciplinary areas related to specific professional subject area of physical sciences, including professional engagement in advanced research and developments.

PO2: Analyse and interpret the scientific truths/information using appropriate methods, including the specific programming skill with the use of appropriate software , and report the findings accurately with experimental results.

PO3: Demonstrate the relevant generic skills and global competencies such as problem solving,investigative skills, analytical skills, communication skillsand ICT skills.

PO4: Develop Entrepreneurship interest with ability to work individually and in a group.

PO5: Assimilate the skills and cognitive developments in explicit areas associated to current and emerging technology concerned with societal, national and global requirements. Validate the professional behavioursuch as being unbiased and truthful in all aspects.

Programme Specific Outcomes (PSO)

After completion of the programme, the students will be able to

PSO1: Understand the chemical concepts, theories, laws and chemistry behind the various analyses related to qualitative and quantitative aspects in the various domains of life. Acquire and apply the subject knowledge and skills in needed situations, i.e., in industrial, research, and professional careers.

PSO2: Understand the various chemical and nuclear reactions, mechanisms involved and applications of the chemical reactions. Apply the knowledge on various chemical reactions to the various industrial research and development processes.

PSO3: Apply the knowledge of different spectroscopic, chromatographic thermo analytical and electroanalytical techniques. Analyse and interpret the experimental results using suitable instrumental techniques and finding the quantitative and qualitative aspects of the analyses and its impacts.

PSO4: Acquire the specific skills like, investigative skill, analytical skill, demonstrative skill and ICT skills. Acquire Entrepreneurship skills, and problem-solving skills to face the competitive examinations and interviews with confidence.

PSO5: Understand and apply the knowledge of laboratory experiments, instrument handling and standard equipment's handling and interpretation ofthe experimentaldata can be extended to various dimensions of professionals such as industry-basedR&D and societal need based scientific problems andto the current and emerging scientific technologies.

M.Sc. CHEMISTRY
SCHEME OF EXAMINATION

SEMESTER- I

S. No.	Course Code	Course Title	Hrs. /Week.	Credits	Exam Hrs.	Max. Marks		
						Int.	Ext.	Total
1	20PCH1C01	Core: Inorganic Chemistry-I (Nuclear and Solid State Chemistry)	5	5	3	50	50	100
2	20PCH1C02	Core: Organic Chemistry-I (Organic Reaction Mechanism-I)	5	4	3	50	50	100
3	20PCH1C03	Core: Physical Methods in Chemistry (Group Theory and Spectroscopy)	5	4	3	50	50	100
4	20PCH1EL1	Elective: Analytical Chemistry	5	4	3	50	50	100
5	20PCH2CP1	Core Practical: Inorganic Chemistry-I	3	-	-	-	-	-
6	20PCH2CP2	Core Practical: Organic Chemistry-I	3	-	-	-	-	-
7	20PCH2CP3	Core Practical: Physical Chemistry-I	4	-	-	-	-	-
Subtotal-I			**30**	**17**		**200**	**200**	**400**

SEMESTER- II

S. No	Course Code	Course Title	Hrs. /Week.	Credits	Exam Hrs.	Max. Marks		
						Int.	Ext.	Total
1	20PCH2C04	Core: Inorganic Chemistry-II (Coordination Chemistry)	5	5	3	50	50	100
2	20PCH2C05	Core: Organic Chemistry-II (Organic Reaction Mechanism-II)	5	4	3	50	50	100
3	20PCH2C06	Core: Physical Chemistry-I (Quantum Chemistry &Spectroscopy)	5	4	3	50	50	100
4	20PCH2EL2	Elective: Polymer Chemistry	5	4	3	50	50	100
5	20PCH2CP1	Core Practical: Inorganic Chemistry-I	3	3	6	50	50	100
6	20PCH2CP2	Core Practical: Organic Chemistry-I	3	3	6	50	50	100
7	20PCH2CP3	Core Practical: Physical Chemistry-I	4	3	6	50	50	100
Subtotal-II			**30**	**26**		**350**	**350**	**700**

SEMESTER- III

S. No	Course Code	Course Title	Hrs. /Wek.	Credits	Exam Hrs.	Max. Marks		
						Int.	Ext.	Total
1	20PCH3C07	Core: Physical Chemistry-II (Thermodynamics)	5	5	3	50	50	100
2	20PCH3C08	Core: Organic Chemistry-III (Chemistry of Natural Products)	5	5	3	50	50	100
3	20PCH3C09	Core: Organic Reactions and Reagents	5	5	3	50	50	100
4	20PCH3EL3	Elective: Computational Chemistry and Molecular Modeling	5	4	3	50	50	100
5	20PCH4CP4	Core Practical: Inorganic Chemistry-II	3	-	-	-	-	-
6	20PCH4CP5	Core Practical: Organic Chemistry-II	3	-	-	-	-	-
7	20PCH4CP6	Core Practical: Physical Chemistry-II	4	-	-	-	-	-
Subtotal-III			**30**	**19**		**200**	**200**	**400**

SEMESTER- IV

S. No	Course Code	Course Title	Hrs/WK	Credits	Exm. Hrs	Max. Marks		
						Int	Ext	Tot
1	20PCH4C10	Core: Physical Chemistry-III (Chemical Kinetics and Electro Chemistry)	5	5	3	50	50	100
2	20PCH4EL4	Elective: Nano Science and Green Chemistry	5	4	3	50	50	100
3	20PCH4EL5	Elective: Medicinal Chemistry	5	4	3	50	50	100
4	20PCH4CPR	Core: Project Work	5	5	-	50	50	100
5	20PCH4CP4	Core Practical: Inorganic Chemistry-II	3	3	6	50	50	100
6	20PCH4CP5	Core Practical: Organic Chemistry-II	3	3	6	50	50	100
7	20PCH4CP6	Core Practical: Physical Chemistry-II	4	4	6	50	50	100
Subtotal-IV			**30**	**28**				**700**
GRAND TOTAL				**90**		**350**	**350**	**2200**

Course Title	**:**	**Core: Inorganic Chemistry-I** (Nuclear and solid-state chemistry)	**Course Code**	**:**	**20PCH1C01**
Year	**:**	**I**	**Semester**	**:**	**I**
Hours/Week	**:**	**5**	**Credit**	**:**	**5**

Course objectives:

Enable the students to

1. understand the basic structure and characteristics of nuclei through nuclear models
2. know the various types of nuclear reactions and understand the working of particle accelerators
3. understand the function and types of nuclear reactors
4. know the various applications of radioactive isotopes
5. understand the crystal structures through diffraction methods
6. gain the knowledge about structure and bonding in inorganic polymers

Course Outcomes

After learning the course, the students will be able to

CO1	describe the basic characteristics of nuclei through nuclear models	K1& K2
CO2	distinguish the various types of nuclear reactions and demonstrate the working principle of particle accelerators.	K2& K4
CO3	analyse themerits and demerits of nuclear energy and discuss the various applications of radioisotopes.	K4& K2
CO4	apply the various diffraction techniques to understand the crystal structures	K3& K4
CO5	explain the chemistry of inorganic polymers	K2

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	M	S	L	M		S	S	M	M	L
CO2	S	S	L	M	M		S	S	M	M	L
CO3	M	S	M	M	M		M	S	M	M	M
CO4	M	S	M	M	S		M	M	M	S	S
CO5	S	M	L	M	M		S	S	M	M	L

S-Strong, M-Medium, L-Low

UNIT–I

Nuclear models: the shell model–the liquid drop model. Units of radioactivity.Alpha decay–range, ionizing power, energy spectrum, Geiger–Nuttal's rule, theories of alpha decay–tunnel effect. Beta decay–types–$\beta^-$and β^+ decay, electron capture, absorption, range and energy. Gamma ray–radiative de–excitation, decay constant, nuclear isomerism, internal conversion, the Auger effect.Artificial radioactivity.

Detection and measurement of radioactivity–proportional counter, G.M. counter, scintillation counter, semiconductor detector, cloud chamber and bubble chamber.

UNIT–II

Nuclear reactions: Bethe's notation. Scattering, photonuclear, evaporation, spallation, fission, fragmentation, stripping and pick–up reactions.Reaction cross section, Q value, threshold energy, and coulombic barrier. Nuclear reactions induced by neutrons and protons. Charged particle accelerators–linearaccelerator, cyclotron, beatatron and bevatron.Types of fission reactions.

UNIT–III

Nuclear energy sources: nuclear fission energy & nuclear reactors, the four factor formula–Classification of reactors–thermal, natural uranium, heavy water, heterogeneous water cooled and PHWR. Critical size of a thermal reactor–Fast Breeder reactor.Energy from nuclear fusion–Stellar energy–thermonuclear reactions on earth–fusion bomb. Applications of radioactive isotopes as tracers, chemical investigations, analytical applications–isotopic dilution, neutron activation–radiometric titration, Libby's C–14 dating method–industrial and medical applications.

UNIT–IV

Solid state chemistry: Ionic crystals–coordination number, radius ratio rule and shapes of ionic crystals–structures of ionic crystals–AX type CsCl, ZnS (Zinc blende and Wurtzite)–AX_2 type calcium fluoride, titanium dioxide, cadmium iodide. Experimental methods of crystal structure determination–X–ray diffraction, electron diffraction and neutron diffraction. Comparative study of the three diffraction methods.

UNIT–V

Inorganic polymers:preparation, structure, reactions and uses of silicone polymers, silicone fluids, gums, elastomers and resins. Phosphonitrilic compounds–trimer and tetramer. Nitrides of sulphur–S_4N_4, $(NSF)_3$, $(NSF)_4$. Isopoly and heteropoly acids of molybdenum and tungsten–preparation, reactions, uses and structures–boranes–Wade's rule–calculation of frame work electrons.

Books for Reference

1. H.J. Arnikar, Essential of Nuclear chemistry, New Age International Publishers, Edn.4 (1997).
2. U. N. Dash, Nuclear Chemistry, Edn. 1 (1971)
3. GurudeepRaj, Advanced Inorganic Chemistry, Vol. I,KrishnaPrakasam Media (P) Ltd., Edn. 25 (1999).
4. B.R. Puri, L.R Sharma and K.C. Kalia, Principles of Inorganic chemistry, Vallabh Publishers (2005).

E-resources:

1. https://www.youtube.com/watch?v=Xs7SFulW4oE
2. https://www.youtube.com/watch?v=bukjtmM2djU
3. https://www.youtube.com/watch?v=6axVVhi62ac
4. https://www.youtube.com/watch?v=d3itX1llkPA
5. https://www.youtube.com/watch?v=vPJidbP_oLM

Course Title	**:**	**Core: Organic Chemistry-I (Organic Reaction Mechanism-I)**	**Course Code**	**:**	**20PCH1C02**
Year	**:**	**I**	**Semester**	**:**	**I**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. gain knowledge on aromaticity, reaction organic mechanisms and reaction intermediates
2. understand the chemistry and mechanism of addition, substitution & elimination reactions of organic compounds
3. analyse the stereochemistry of the products formed in various reactions.

Course Outcomes

After learning the course, the students will be able to

CO1	explain the concept aromaticity andpredict the aromaticity of compounds.	K1& K2 K3
CO2	elaborate the mechanisms involved and the corresponding reactions of aromatic electrophilic substitution reactions and aromatic nucleophilic substitution reactions.	K2
CO3	describe the mechanism, orientation and reactivity of aliphatic nucleophilic substitution reaction.	K2 &K4
CO4	distinguish the nucleophilic, electrophilic and free radical mechanisms of elimination reactions.	K2& K4
CO5	explain the mechanisms and stereochemistry of elimination reactions.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	S	S	M	M	M		S	S	M	M	L
CO3	S	S	M	L	M		S	S	M	L	M
CO4	S	S	M	M	L		S	S	M	M	L
CO5	S	S	M	M	M		S	S	M	M	M

S-Strong, M-Medium, L-Low

UNIT–I

Aromaticity–benzenoid and non-benzenoid aromatics–ferrocene, azulene and annulenes.Alternant and non-alternant hydrocarbons–homoaromaticity–antiaromaticity.Kinetic and non-kinetic methods of study of reaction mechanisms–primary kinetic isotopic effect, study of intermediates, isotopic labelling and cross over experiments.Hammond's postulates.Linear free energy relationship–Hammet equation.

UNIT–II

Arenium ion mechanism–orientation and reactivity of mono and disubstituted benzenes.Aromatic electrophilic substitution reactions.Formylation–Gattermann, Gattermann Koch, Reimer–Tiemann, Kolbe, Bischler–Napieralski, Hoffmann–Maritus and Jacobsons reactions.Friedel–Crafts alkylation

and acylation.Aromatic nucleophilic substitution reactions–Benzyne mechanism–Intermediate complex mechanism and SNAr mechanism–structure reactivity relationship–Ziegler alkylation and Chichibabin reaction.

UNIT–III

Aliphatic nucleophilic substitution reactions–S_N1, S_N2, S_Ni, S_N1', S_N2' and S_Ni' mechanisms, substitution at vinyl carbon–stereochemistry of nucleophilic substitution reaction–effect of substrate structure–solvent effect–leaving group effect–nucleophilicity–ambident nucleophiles and ambident substrates, neighbouring group participation. Aliphatic electrophilic substitution reactions–S_E1, S_E2 and$S_E$imechanisms, structure reactivity relationship.Friedel Crafts acylation at olefinic carbon–Stork–enamine reaction.

UNIT–IV

Electrophilic, nucleophilic and free radical addition reaction to double and triple bonds–Hydration, hydroboration, Michael addition, epoxidation and hydroxylation. Addition reactions to carbonyl compounds–Mannich reaction–MeerweinPonndorff–Verley (MPV) reduction–addition of Grignard reagents to aldehydes and ketones–Claisen, Dieckmann, Stobbe, Knoevenagel, Darzen, Wittig, Thorpe and Benzoin reactions.

UNIT–V

Elimination reactions: E1, E2, Ei, $E1_CB$ mechanisms, stereochemistry of elimination reactions, effect of substrate structure, effect of attacking base, effect of leaving group, effect of medium and eliminations vs substitution. Typical elimination reactions–Chugaev reaction, Hoffmann degradation, Cope elimination and dehydration of alcohols.Carbenes and nitrenes–structure, generation and reactions.

Books for study and Reference

1. Jerry March, Advanced Organic Chemistry, (Reaction Mechanism and structure). McGraw Hill Gogakusha, New Delhi (1977)
2. I. L. Finar Organic Chemistry, ELBS, Edn V (1975)
3. R. L. Morrision and R. N. Boyd, Organic Chemistry,Prentice Hall of India Pvt Ltd, Edn. VI (1992).
4. Badger, Aromaticity and Aromatic Character,Cambridge University Press (1969)
5. Petersykes Guide book to mechanisms in Organic Chemistry,OrientLongmann (1986)
6. Jagadamba Singh and L.D.S.Yadav, Advanced Organic Chemistry, PragatiPrakashan (2004).

E-resources:

1. https://byjus.com/chemistry/aromaticity/
2. https://www.youtube.com/watch?v=pvyvtYsnU2s&t=245s
3. https://www.youtube.com/watch?v=-OxgknhtrYI
4. https://www.youtube.com/watch?v=nl-tZR0u96s
5. https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1b.htm#indxb

Course Title	**:**	**Core: Physical Methods in chemistry** (Group theory and spectroscopy)	**Course Code**	**:**	**20PCH1C03**
Year	**:**	**I**	**Semester**	**:**	**I**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course objectives:

Enable the students to

1. enhance the knowledge on symmetry of the molecules and its applications
2. educate about the applications of group theory
3. enrich the knowledge on IR spectroscopy
4. transfer the knowledge on the applications of UV-Vis spectroscopy
5. inculcate the significance of mass spectrometry

Course Outcomes

After learning the course, the students will be able to

CO1	recognise the various symmetry elements of molecules.	K1 &K2
CO2	explain the applications of group theory	K1 &K2
CO3	describe the principle, theory and applications of infrared spectroscopy.Identify the IR spectrum of unknown organic compounds.	K2 K3& K4
CO4	elaborate the theory involved in UV-Visible absorption spectroscopy. Identify the UV-Vis spectrum of unknown compounds.	K2 & K3 K4
CO5	explain the fragmentation pattern, detection of various ions , various peaks and instrumentation of mass spectrometry. Predict the fragmentation patterns for new compounds.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	S	S	M	M	M		S	S	M	M	L
CO3	S	S	S	M	M		S	M	S	M	M
CO4	S	S	S	M	M		S	M	S	M	M
CO5	S	S	S	M	M		S	M	S	M	M

S - Strong, M- Medium, L-Low

UNIT–I

Symmetry elements and symmetry operations.Inverse operations. Definition of a group–properties of a group, definition of abelian group, cyclic group, finite group, infinite group, sub–group and isomorphic group–group multiplication tables. Symmetry classification of molecules into point groups (Schoenflies symbols only).

Matrices: Definition of matrix, diagonal matrix, null matrix, unit matrix, row matrix, column matrix, symmetric matrix, skew matrix and conjugate matrix. Matrix

multiplication.Determinationofinverse matrix. Block multiplication of matrices. Matrix notations of symmetry operations of C_{2V} and C_{3V} point groups.

UNIT–II

Definition of reducible and irreducible representations. Direct product rule. The great orthogonality theorem and its consequences(statement only proof not needed). Construction of character table for C_{2V}& C_{3V} point groups. Calculation of character values of reducible representation per unshifted atom for each type of symmetry operation. Determination of total Cartesian representation.

Group Theory and Vibrational Spectroscopy: Vibrational modes as bases for group representations. Symmetry selection rules for IR and Raman spectra(mutual exclusion principle). Classifications of vibrational modes.

Applications of group theory to bonding: Hybridization schemes for orbitals in AB_3(planar).$AB_4(T_d)$, $AB_5(D_{3h})$, $AB_6(O_h)$ types of molecules. Hybridization schemes for bonding in $AB_3(D_{3h})$ and $AB_6(O_h)$ types of molecules. Group theory and dipole moment.

UNIT–III

IR Spectroscopy–Theory–IR region. Molecular vibrations–calculation of vibrational frequency.Number of fundamental vibrations–selection rules–factors influencing vibrational frequencies–instrumentation–Finger print region–identification of functional groups–application of IR spectroscopy to simple organic molecules. The Raman effect–Stoke's and antistoke's lines. Comparison between IR and Raman spectra.

UNIT–IV

Ultraviolet and visible spectroscopy Theory, Beer and Lambert's laws.Types of electronic transitions–selectionrules–Franck–Condon principle.Born–Oppenheimer Approximation.Designation of bands(R, K and B bands) Chromophores and auxochromes. Bathochromic, hypsochromic, hyperchromic and hypochromic shifts.

Photometric titrations. Woodward–Fieser rules for calculating absorption maximum of dienes, polyenes and α, β–unsaturated carbonyl compounds.

UNIT–V

Mass Spectrometry–Presentation of mass spectrum–instrumentation–sample insertion, ion source, mass analyzer and ion detectors. Resolution.Types of ions–molecular ion, fragment ion, rearrangement ion, metastable ion, odd and even electron ions. Molecular ion peak, base peak and metastable ion peak.Nitrogen Rule, Isotope abundances.Fragmentation of aldehydes and ketones, alcohols, phenols, carboxylic acids and amines.Retro–Diels Alder Reaction.McLafferty rearrangement. Double bond and ring equivalence.

Books for study and Reference

1. F.A. Cotton, Chemical applications of group theory, Wiley Eastern Ltd Edn. 2, (1988).
2. R.M. Silverstein, G. Clayton Bassler, and Terence C. Morril, Spectrophotometric identification of organic compounds. John Wiley & sons Edn. 5. (1991).
3. F. Sheinmann, An introduction to spectroscopic methods for identification of organic compounds, Vol. I & II by, Pergamon Press(1970)
4. C.K. Banwell,Fundamentals of molecular spectroscopy, Tata McGraw Hill(1983).

5. W. Kemp Organic Spectroscopic, ELBS, Edn.3 (1991).
6. Das and James,Organic Mass Spectroscopy, Oxford GBH Publishing, New Delhi (1976).
7. P.S. Kalsi, Spectroscopy of organic compounds, Wiley Eastern Ltd.
8. Jag Mohan, Organic Spectroscopy–principles and applications II Edition Narosa Publishing House Pvt. Ltd.
9. K.Veera Reddy, Symmetry and Spectroscopy of molecules, New Age International (1998).
10. Y. R. Sharma, Elementary organic spectroscopy, S. Chand & Co (2007)

E-resources:

1. https://freevideolectures.com/course/4859/nptel-chemical-applications-symmetry-group-theory
2. https://freevideolectures.com/course/4330/nptel-infrared-spectroscopy-pollution-monitoring/14
3. https://www.youtube.com/watch?v=Vl3BYsoif-c
4. https://www.khanacademy.org/science/organic-chemistry/spectroscopy-jay/uv-vis-spectroscopy/v/uv-vis-spectroscopy
5. https://www2.chemistry.msu.edu/faculty/reusch/virttxtjml/spectrpy/spectro.htm

Course Title	**:**	**Elective: AnalyticalChemistry**	**Course Code**	**:**	**20PCH1EL1**
Year	**:**	**I**	**Semester**	**:**	**I**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. learn the thermal methods of analyses.
2. enrich about the concepts and applications of polarimetry.
3. teach the principles and instrumentations of atomic absorption spectrometry.
4. impart the theories and applications of chromatographic techniques.
5. enable the students the analyse the analytical data

Course Outcomes

After learning the course, the students will be able to

CO1	investigate the thermal properties of the sample throughthermal studies.	K3& K4
CO2	analyse and identifythe optical property of the sample through polarimetry, ORD and CD techniques.	K3& K4
CO3	explain theprinciple and working of AAS and FES.Distinguish both the techniques.	K1 & K2 K4
CO4	demonstrate the various chromatographic techniques.	K1& K2
CO5	Analyse andvalidate the experimental data.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	M	M	S	S	M		M	S	S	M	M
CO2	M	S	S	M	M		M	S	S	M	M
CO3	S	S	M	L	M		S	S	S	L	M
CO4	M	M	S	S	L		M	S	M	S	L
CO5	M	S	S	S	L		M	S	S	M	L

S-Strong, M-Medium, L-Low

UNIT–I

Thermal methods of analysis: principle, instrumentation and applications of thermogravimetry, differential thermal analysis and differential scanning calorimetry,–thermometric titrations. Refractometry–theory, Abbe's refractometer and applications of refractometry.

UNIT–II

Polarimetry–Plane polarised light–optical activity of molecules–polarimeter and its uses. ORD and CD spectrometry, circular birefringence, circular dichroism , optical rotatory dispersion , plain curves , anomalous curves–Cotton effect–axial haloketone rule and octant rule–application.Nephelometry and Turbidimetry–principle, instrumentation and applications.

UNIT–III

Atomic Absorption Spectrometry: principle–instrumentation–detection of metals & non–metals, interference, detection limit & sensitivity and applications.

Flame Emission spectrometry–Principle, instrumentation, methodology and applications. Comparison between AAS and FES.

Molecular fluorescence and phosphorescence–theory, instrumentation and applications.

UNIT–IV

Chromatographic methods: Basic principles, theories, instrumentation, experimental procedures and application of following chromatographic techniques–paper, thin layer, column, gas chromatography, high performance liquid chromatography and ion–exchange chromatography.

UNIT–V

Significant figures, errors–determinate and indeterminate, precision, mean, median, mode, average deviation, standard deviation (sample and population)–relative standard deviation–accuracy, difference between precision and accuracy, propagation of determinate errors, reporting of analytical data–uncertainty, statistical treatment of analytical data–Confidence limits, Student's t–values for various probability levels and varying degrees of freedom. Rejection of a result–Q–test, tests of significance–F–test and t–test.

References

1. B.K. Sharma, Chromatography , Goel Publishing House.(2004)
2. Gurdeep R. Chatwal& S.K. Anand, Instrumental Methods of Chemical Analysis, Himalaya Publishing House (2003) .
3. B.K. Sharma, Instrumental Methods of Chemical Analysis, Goel Publishing House (2003).
4. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International Publishers.(2010).
5. B.R.Puri, L.R. Sharma and K.C.Kalia, Principles of Inorganic Chemistry, Milestone Publishers (2010).
6. Larry G.Hargis, Analytical chemistry, Prentice Hall(1988).

E-resources:

1. https://www.youtube.com/watch?v=qIFdQNXjJ7k&list=RDCMUC_MZLIpJljWvJ0m092bm6Ug&index=21
2. https://www.youtube.com/watch?v=m8LSsdRafLo
3. https://freevideolectures.com/course/3029/modern-instrumental-methods-of- analysis/42
4. https://freevideolectures.com/course/2380/chemistry-laboratory-techniques
5. https://freevideolectures.com/course/3025/novel-separation-processes

Course Title	**:**	**Core: Inorganic Chemistry - II** (Coordination Chemistry)	**Course Code**	**:**	**20PCH2C04**
Year	**:**	**I**	**Semester**	**:**	**II**
Hours/Week	**:**	**5**	**Credit**	**:**	**5**

Course Objectives:

Enable the students to

1. boost the knowledge on coordination chemistry
2. know about the electronic spectra of Inorganic compounds
3. enrich the knowledge on organometallic compounds
4. learn the basic concepts of Bio-Inorganic chemistry
5. imbibe the catalytic applications of organometallic compounds

Course Outcomes

After learning the course, the students will be able to

CO1	comprehend the theories of coordination chemistry and understand its application.	K1& K2
CO2	analyse the various aspects of electronic spectra of inorganic complexes.	K2& K4
CO3	discuss the chemistry of organometallic compounds. Apply infrared spectroscopy to study organometallic compounds	K2 & K4
CO4	understand and analyse the ligand substitution reactions	K3& K4
CO5	explain the catalytic applications of organometallic compounds	K1& K2

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	S	S	M	M	L		S	S	M	M	L
CO3	S	S	S	L	M		S	S	M	L	M
CO4	S	S	M	M	L		S	S	M	L	M
CO5	S	S	M	M	L		S	S	M	M	L

S-Strong, M-Medium, L-Low

UNIT–I

Bonding in coordination complexes: Crystal field theory (CFT)–crystal field splitting in octahedral, tetrahedral and square planar complexes, factors affecting crystal field stabilization energy (CFSE)–spectrochemical series–magnetic and spectral properties, colours of transition metal complexes–applications of CFSE. Molecular orbital Theory (MOT)–MO diagrams of octahedral, tetrahedral and square planar symmetries. Experimental evidences for pi–bonding.

UNIT–II

Electronic spectra of transition metal complexes: Derivation of Term symbols to P^2 and d^2, spin–spin and spin orbit couplings–selection rules and relaxations–splitting of electronic energy levels and spectroscopic states–Orgel Diagram–interpretation of electronic spectra of d^1 to d^9 metal ions–Tanabe–Sugano diagrams of d^2 and d^3 systems. Jahn–Teller tetragonal distortions–Nephelauxetic effect. Charge transfer spectra.

UNIT–III

Chemistry of pi–acceptor ligand complexes: Preparative methods, reactions, structure and bonding of transition metal carbonyls, carbonyl hydrides, carbonyl halides, nitrosyls, and dinitrogen complexes. Applications of IR spectroscopy to metal carbonyls. Organometallic compounds: preparation, structure and bonding in metal–alkenes, alkyne, allyl and butadiene complexes. Metallocenes: preparation, properties and bonding in ferrocene. Preparation and structure of arene complexes formed by seven and eight membered rings.

Unit–IV

Complexes of biochemical importance: structure and functions of Cytochromes, Myoglobin and Hemoglobin, Ferredoxins, Chlorophyll and Cyanocobalamin(Vitamin B_{12}).

Ligand substitution reactions in octahedral complexes: Types of substitution reactions–mechanism of S_N1 and S_N2 reactions, acid and base hydrolysis reactions–S_N1_CB mechanism. Anation reactions.

UNIT–V

Ligand substitution reactions in square–planar complexes: Trans effect–theories of trans effect, applications of trans effect–mechanism of substitution reactions in square–planar complexes. Complementary electron transfer reactions. Catalysis by organometallic compounds–alkene hydrogenation (Wilkinson's catalyst), hydroformylation(oxoproces), Monsanto acetic acid process, the Wacker process and Ziegler–Natta catalysis.

References

1. J.E. Huheey, E.A. Keither and R.L. Keither, Inorganic chemistry, Harper Collins College Publishers, Edn 4(1993).
2. J.D. Lee, Concise Inorganic chemistry, Blackwell science Edn. 2 (1996).
3. W.U. Malik, G.D.Tuli and R.D. Madan, Selected Topics in Inorganic Chemistry, S.Chand& Co. (2004).
4. Gurdeep Raj, Advanced Inorganic Chemistry Vol–II, Goel Publishing House (2004).
5. F.A. Cotton and G. Wilkenson, Advanced Inorganic Chemistry Wiley & Sons.Edn.6 (2006).
6. H.J. Emeleus and A.G. Sharpe Modern Aspects of Inorganic Chemistry, ELBSEdn. 4 (1973).

E-resources:

1. https://freevideolectures.com/course/3412/co-ordination-chemistry
2. https://www.youtube.com/watch?v=QOEUYsDCtnY
3. https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm
4. https://freevideolectures.com/course/3371/introduction-to-organometallic-chemistry
5. https://www.youtube.com/watch?v=pXztk04J7u0&list=PLFW6lRTa1g83-gUOcT3ay875UG3a9Mu11

Course Title	**:**	**Core: Organic Chemistry-II** (Organic Reaction Mechanism -II)	**Course Code**	**:**	**20PCH2C05**
Year	**:**	**I**	**Semester**	**:**	**II**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. learn the salient features, utility, and understand the conservation of orbital symmetry in pericyclic reactions.
2. enable the students to understand the mechanistic aspects of photo-induced reactions and photo-physical processes.
3. understand the chemistry and mechanism of oxidation and reductions reactions.
4. imbibe the modern concepts of acid and bases and their applications in view of organic chemistry.
5. make the students to understand the effect of conformation on chemical reactivity.

Course Outcomes

After learning the course, the students will be able to

CO1	analyse and predict the various pathways for the synthesis of new organic compounds with specific stereochemistry.	K3& K4
CO2	explain the photophysical and photochemical pathways of an excited species.	K1 & K2
CO3	apply the suitable oxidizing and Reducing reagents for wide range of functional groups	K4
CO4	understand and analyse the concepts of acid-bases and their applications.	K2& K3
CO5	analyse the effects of various conformations on chemical reactivity.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	M	S	S	M	L		M	S	S	M	L
CO2	S	S	M	M	L		S	S	M	M	L
CO3	M	S	S	L	M		M	S	S	L	M
CO4	S	S	M	M	L		S	S	L	M	M
CO5	S	S	M	M	L		S	S	M	M	L

S-Strong, M-Medium, L-Low

UNIT–I

Pericyclic reactions: Electrocyclic reactions–molecular orbital correlation diagram and frontier molecular orbital (FMO) theory applicable to the electrocyclic conversion of 1,3–dienes and 1,3,5–trienes, [2+2] cycloadditions and [2+4] cycloadditions. Sigmatropic rearrangements–[1,5] sigmatropic rearrangement, Claisen and Cope rearrangements. The perturbation theory of pericyclic reactions. Di–π–methane rearrangement, ene reactions and 1, 3–dipolar additions.

UNIT–II

Photochemistry: Introductory theory of light absorption–Jablonski diagram, dissipation of excess energy of the excited molecules, radiative transitions–fluorescence, phosphorescence, delayed fluorescence–e–type and p–type. Radiative transitions involving more than one molecule–excimers, exciplexes. Radiationless transitions involving internal conversion and intersystem crossing, energy transfer–intermolecular and intramolecular–photosensitisation and quenching. Photochemical reactions of ketones–Paterno–Buchi reaction, Norrish type I and type II reactions, cis–trans isomerization, photoreduction and photo oxidation.

UNIT–III

Oxidation by chromic acid, manganese (IV) oxide, silver carbonate, dimethyl sulphoxide, dess–Martin periodinane oxidation, Oxidations of carbon–carbon double bonds–epoxides, enantioselectiveepioxidation of allylic alcohols (sharpless asymmetric epoxidation)–diastereo selective epoxidation of homo allylic alcohols, m–chloroperbenzoic acid and osmium tetroxide, Prevost reaction, catalytic hydrogenation, selectivity of reduction, reduction of functional groups (alkenes, alkynes, aldehydes and ketones), stereochemistry and mechanism, homogeneous hydrogenation.

Reduction by dissolving metals–metal and acid, metal and alcohol. Reduction by hydride transfer reagents–di–isobutyl aluminium hydride (DIBAL), alkoxy, alkyl and acyloxyborohydrides. Metal catalysed Carbon–Carbon bond forming reaction–Suzuki and Hech coupling.

UNIT–IV

Acids and Bases: Arrhenius theory, Bronsted theory, acidic and basic solvents, levelling effect, measurement of solvent acidity, acid and base catalysis, Lewis acids and bases. Effect of structure on strength of acids and bases–inductive effect–resonance effect–state of hybridization.Effect of medium on acid and base strength.Hard and soft acids and bases.HSAB Principle–MO theory and applications of HSAB theory.

UNIT–V

Conformational analysis and stereochemistry: Conformations of cyclohexane, substituted cyclohexanes and decalins. Conformation and reactivity in substituted cyclohexanes.Assignment of R and S configuration in chiral non–racemic molecules.Stereochemistry of biphenyls, allenes and spiranes.Stereochemistry of sulphur and nitrogen compounds.Stereochemical reagents in organic reactions–Wilkinson catalyst, *t*–C_4H_9 COOH, (+)n diethyl tartrate, di–isopropyl tartrate and tetra isopropyltitanium

References

1. Jerry March, Advanced Organic Chemistry (Reaction Mechanism and Structure). McGraw Hill Gogakusha, New Delhi (1977)
2. E. L. Eliel Stereochemistry of Carbon compounds, Tata McGraw Hill (1962)
3. C.H.Depuy and O. C. Chapman, Molecular reactions and Photochemistry, Prentice Hall (1975)
4. S. Muherjee and S. P. Singh, Reaction Mechanisms in Organic Chemistry (1976)
5. R. K. Bansal, Organic reaction mechanisms, Tata McGraw Hill, Edn. 2 (1986)
6. K. Nasipuri, Stereochemistry of Organic Compounds–Principles and applications, Wiley Eastern Limited (1992).
7. W.M.Horspool, Aspects of Organic Photochemistry, Academic Press (1976)
8. Jagadamba Singh, Photochemistry and Pericyclic reactions, New Age Int.Pvt.Ltd. (2003)

9. I.L. Finar, Organic Chemistry Vol–II, Stereochemistry and the Chemistry of Natural Products, ELBS, 5th Edition
10. N. Tewari, Advanced Organic Stereochemistry (Problems and Solutions) (2010)

E-resources:

1. https://freevideolectures.com/course/3125/organic-photochemistry-and-pericyclic-reactions
2. https://freevideolectures.com/course/3125/organic-photochemistry-and-pericyclic-reactions
3. https://ocw.mit.edu/courses/chemistry/5-111-principles-of-chemical-science-fall-2008/video-lectures/lecture-21/
4. https://nptel.ac.in/courses/104/105/104105086/
5. https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1b.htm#indxb

Course Title	**:**	**Core: Physical Chemistry-I** (Quantum Chemistry and Spectroscopy)	**Course Code**	**:**	**20PCH2C06**
Year	**:**	**I**	**Semester**	**:**	**II**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. make students aware about the basic formulations in quantum chemistry. There are many different types of representations of state and operators that are very useful in studying the subject deeply.
2. give information about hermitian operators, their eigenvalues and eigenfunctions. It teaches about various commutation and uncertainty relations.
3. insight to solve Schrodinger wave equation of a particle in one, two and three dimensions boxes.
4. solve Schrodinger wave equation for Rigid rotor and Linear harmonic oscillator and calculate their respective energies.
5. know the basic ideas and applications of Mossbauer and NMR spectroscopic methods.

Course Outcomes

After learning the course, the students will be able to

CO1	describe the types of representations of operators and apply them in different problems.	K3& K4
CO2	distinguish time independent degenerate and non-degenerate perturbations and to apply them in various problems.	K4 & K3
CO3	explain the need for approximation methods. Discuss the applications of these methods.	K1 & K2
CO4	predict the ESR spectrum of new compounds.	K3& K4
CO5	identify the NMR spectrum of the unknown compounds.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	M	S	L	M		M	S	S	L	M
CO2	M	S	S	M	L		M	S	S	M	L
CO3	S	S	M	L	M		S	S	M	M	L
CO4	M	S	S	L	M		S	S	S	M	M
CO5	M	S	S	M	L		M	S	S	M	L

S-Strong, M-Medium, L-Low

UNIT I

Blackbody radiation–failure of classical theories (Wein law and Rayleigh–Jeans law only) Planck's quantum theory in explaining blackbody radiation. Einstein's theory of photoelectric effect.

H–atomic spectrum–de–Broglie hypothesis.Heisenberg's uncertainty principle.Time–dependent and time–independent Schrodinger equations–interpretation of wave function and requirements of wave functions.Operators–addition and subtraction, product of operators, commutator and linear operator.

Eigen functions and Eigen values. Correspondence between physical quantities and operators.Hamiltonian and angular momentum operators.Postulates of quantum mechanics.

UNIT II

Treatment of particle in one dimensional box–quantization of energy, normalization of wave function, orthogonality of a particle in one dimensional box–illustration of uncertainty principle for a particle in one dimensional box, particle in a three dimensional box–principle of separation of variables. Harmonic oscillator model of a diatomic molecule–finding asymptotic solution of Schrodinger equation for a one dimensional harmonic oscillator.Rigid rotator model of a diatomic molecule–solving the Φ equation of Schrodinger equation of the rigid rotator. H–atom (H like species) (solving radial and θ equations not necessary). Shapes of orbitals.

UNIT III

Electron spin–He–atom–Pauli exclusion principle–anti symmetric wave functions.Approximate wave functions for many electron atoms. Need for approximation methods–perturbation (first order only) and variation methods, applications of perturbation method to Heatom, application of variation method to He atom. Born–Oppenheimer approximation–Hamiltonian operator for a hydrogen molecule using Born–Oppenheimer approximation.

UNIT IV

Mossbauer spectroscopy–Principle, Instrumentation, isomer shift, quadruple interaction, nuclear Zeeman splitting and applications.

ESR theory–instrumentation,derivative curves, 'g' shift, hyperfine splitting,isotropic and anisotropic systems, zero field splitting and Kramer's degeneracy, applications of ESR spectroscopy.

UNIT–V

NMR–Spectroscopy–theory–instrumentation–FT NMR, chemical shift–factors influencing chemical shift, chemical and magnetic equivalence–correlation data, influence of restricted rotation, solvents used–spin–spin coupling–factors influencing coupling constant, proton exchange reactions, hetero nuclear coupling–deuterium exchange, simplification of complex spectra–increased field strengths–double resonance–lanthanide shift reagents, applications of NMR to simple organic molecules, 2D NMR–basic concept–COSEY spectrum, C^{13} NMR–double resonance–nuclear Overhauser effect (NOE)–off resonance decoupling, proton noise decoupling–basic ideas only, comparison between C^{13} and H^{1} NMR.

Books for Reference

1. Silverstein, Bassler and Morril Spectroscopy identification of organic compounds, Hohn Wiley.
2. F. Sheinmann An introduction to Spectroscopic methods for the identification of Organic CompoundsVol I&Vol II ,Pergamon Press, Edn. 1 (1973).
3. R.S.Drago Physical methods in inorganic chemistry
4. K. L. Pavia and G. M. Lapmann. Introduction to Spectroscopy .
5. P. S. Kalsi Spectroscopy of organic compounds , Wiley Eastern Ltd (1971).
6. B.K. Sen, Quantum Chemistry including molecular spectroscopy, Tata McGraw Hill Edn(1992).
7. R. K. Prasad,Quantum Chemistry , New Age Publishers(1994).

8. Donald A. McQuarrie, Quantum Chemistry, Oxford University Press.

E-resources:

1. https://freevideolectures.com/course/3325/introductory-quantum-chemistry
2. https://www.youtube.com/watch?v=Q2Fo5BAReGo
3. https://freevideolectures.com/course/4883/nptel-principles-applications-nmr- spectroscopy
4. https://www.youtube.com/watch?v=Q1GP1PktTEQ
5. https://www.youtube.com/watch?v=TXW0T3RhbRE

Course Title	**:**	**Elective: Polymer Chemistry**	**Course Code**	**:**	**20PCH2EL2**
Year	**:**	**I**	**Semester**	**:**	**II**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. enable the students to learn the basic concepts and classification of polymers impart knowledge about polymerization techniques/mechanism and kinetics of polymerization
2. study the stereochemistry and molecular weight determination methods of polymers
3. learn the different polymer processing techniques and technology of polymers
4. acquire the knowledge on the applications of polymers in various fields.

Course Outcomes

After learning the course, the students will be able to

CO1	distinguish thevarious mechanisms of polymerization andrelate the stereochemistry of polymers with properties	K2& K3
CO2	appreciate the determination the molecular weight of polymers by various methods.	K3
CO3	analyse thermal properties and its significance in the application of polymers.	K4
CO4	demonstrate the different polymer processing techniques.	K1& K2
CO5	understand the properties of speciality polymers and their specific applications.	K1& K2

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	M	S	S	M	L		M	S	S	M	L
CO3	S	S	M	L	M		S	S	M	L	M
CO4	S	S	M	M	M		M	S	M	M	M
CO5	S	S	M	M	L		S	S	M	M	L

S-Strong, M-Medium, L-Low

UNIT I

Mechanism of Polymerisation–Functionality of monomers, classification of polymers, degree of polymerisation and stereoregularity of polymers–isotactic, syndiotactic and atactic.Polymerisation mechanisms–step and addition (kinetics not required).Ring–opening polymerisation and mechanisms of Ziegler–Natta Polymerisation.

UNIT II

Polymerisation Techniques–Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation.

Molecular weight and size: number average and weight average molecular weights. sedimentation and viscosity average molecular weights. Determination of molecular weights.–gel permeation chromatography, end group analysis, viscometry and sedimentation velocity methods.

UNIT III

Thermal properties–glass transition temperature (T_g)–crystalline melting point (T_m)–relationship between T_m and T_g, transitions associated properties–factors affecting T_g–its relationship with molecular weight and melting point. Effects of plasticizers and copolymerisation on T_g.

Reactions of Polymer–Hydrolysis, hydrogenation and cyclisation reactions.Polymer degradation–Thermal, photo and oxidative degradations.

UNIT IV

Technology of Polymers–Processing techniques–calendaring, die casting, rotational casting, film casting, compression, injection, blow and extrusion moulding methods. Fibre technology–textile and fibre properties, spinning, fibre after treatment.Elastomer technology–Natural rubber, chemistry of vulcanisation, reinforcement, elastomer properties and compounding.
Polymer additives–fillers, plasticisers, antioxidants, colorants, flame retardants and stabilizers.

UNIT V

Specialty Polymers: Conducting polymers, liquid crystalline polymers, photopolymers, electroluminescent polymers, polymers for electronic and biomedical applications. Basics of polymer composites.
Miscellaneous Polymers: Methods of preparation, properties and uses of–Teflon, PMMA, Polyethylene, Polystyrene, PAN, Polyesters, Polycarbonates, Polyamides, Polyurethanes, PVC, Buna rubbers, Neoprene rubbers, Epoxy resins, Phenol–formaldehyde and Urea–formaldehyde resins.

Books for study and Reference

1. V.R Gowariker, N.V. Viswanathan and JayadevSreedhar, Polymer Science, New Age International (2010).
2. F. W. Billmeyer, Text Books of Polymer Science, John Wiley and sons (2003).
3. J. R. Fried, Polymer Science and Technology, Prentice Hall (2003).
4. PremamoyGhosh, Polymer Science and Technology of Plastics and Rubbers, Tata McGraw–Hill (2002).
5. A.L.Gupta, Polymer Chemistry, PragatiPrakashan (2010).

E-resources:

1. https://freevideolectures.com/course/3348/polymer-chemistry
2. https://www.youtube.com/watch?v=hsEl7GquggA
3. https://www.youtube.com/watch?v=jSNlmOwpxYg
4. https://www.youtube.com/watch?v=cvI4zLk5OeA
5. https://www.youtube.com/watch?v=r7zYD_DhhtM&list=PLEbdbXWE8jWyDB_ uxEUoa0S 5qF0y1vgrx

Course Title	**:**	**Core Practical: Inorganic Chemistry-I**	**Course Code**	**:**	**20PCH2CP1**
Year	**:**	**I**	**Semester**	**:**	**I & II**
Hours/Week	**:**	**3**	**Credit**	**:**	**3**

Course Objectives:

Enable the students to

1. enhance the skill of Inorganic qualitative analysis
2. elevate the skill on the preparation of Inorganic compounds
3. intensify the skill on colorimetric estimations

Course Outcomes

After learning the course, the students will be able to

CO1	identify the common and less common cations.	K1 & K2
CO2	prepare inorganic complexes.	K2&K3
CO3	estimate colorimetrically the metal ions.	K3&K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	S	S	M		S	S	S	M	M
CO2	M	M	S	S	M		M	M	S	S	M
CO3	M	M	S	S	M		M	S	S	S	M

S-Strong, M-Medium, L-Low

A. Semimicro qualitative Analysis of a mixture containing two common and two less common cations like Thallium, Tungsten, Selenium, Tellurium, Molybdenum, Cerium, Thorium, Zirconium, Vanadium, Beryllium and Lithium.

B.Preparation of the inorganic complexesTris(thiourea)copper(II) sulphate dihydrate,Potassiumtrioxalatochromate(III), Hexathiourealead(II) nitrate, Potassium trioxalatoaluminate(III), Tristhioureacopper(I) chloride.

C. Colorimetric estimations (using photoelectric colorimeter)
Copper, Iron, Nickel, Manganese and Chromium.

References

1. V. V. Ramanujum, Semimicro Qualitative Inorganic Analysis.
2. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, Principles of Practical Chemistry, Sultan Chand & Sons.
3. S. Giri, D. N. Bajpai. and O. P. Panday, Practical Chemistry Vol. I & II S. Chand & Company.

Course Title	**:**	**Core Practical: Organic Chemistry-I**	**Course Code**	**:**	**20PCH2CP2**
Year	**:**	**I**	**Semester**	**:**	**I & II**
Hours/Week	**:**	**3**	**Credit**	**:**	**3**

Course Objectives:

Enable the students to

1. know the separationand analysis of two component organic mixtures.
2. know the chemistry behind the organic qualitative analysis.
3. learn the advantages of green chemistry methods in organic chemistry over conventional methods.
4. know the synthesis of important compounds through named reactions.

Course Outcomes

After learning the course, the students will be able to

CO1	separate and analyse the organic components of a mixture.	K3 &K4
CO2	prepare organic compounds by applying green synthetic methods.	K3 & K4
CO3	prepare organic compounds using organic named reactions.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	M	S	S	M	M		M	S	S	M	M
CO2	M	S	S	M	M		M	S	S	M	M
CO3	M	S	S	M	M		M	S	S	M	M

S-Strong, M-Medium, L-Low

A. Analysis of two component organic mixtures.

Separation and identification of compounds.

B.Green synthesis involving the following reactions using Microwave oven and Sonicator.

Acylation, halogenation, hydrolysis, reduction, oxidation, Schiff base preparation and Chalcones preparation.

C.Preparation illustrating the following reactions.

Cannizzaro reaction, Perkin reaction, Reimer–Tiemann reaction, Sandmeyer reaction, Skraup synthesis, Nitration and Acylation.

D. Preparation illustrating the following rearrangement.

Fries rearrangement

References

1. B. B. Day and M. V. Sitaram and T. R Govindachari, Laboratory Manual of Organic Chemistry. Allied Publishers Limited.
2. Gnanprakasam and Ramamurthy, Organic Chemistry Laboratory Manual, Ananda Book, Depot, Chennai.
3. Jagmohan, Advanced Practical Organic Chemistry, Vol. I & II.

Course Title	**:**	**Core Practical: Physical Chemistry-I**	**Course Code**	**:**	**20PCH2CP3**
Year	**:**	**I**	**Semester**	**:**	**I & II**
Hours/Week	**:**	**3**	**Credit**	**:**	**3**

Course Objectives:

Enable the students to

1. know the method of determining molecular weight of unknown organic compounds by Rast micro method.
2. determine the composition of unknown organic compounds by constructing phase diagram of known organic compounds.
3. facilitate the students to understand the principles behind the potentiometric titrations and carryout the experiments to determine the pH and pKa of some buffer solutions and weak acids respectively.

Course Outcomes

After learning the course, the students will be able to

CO1	determine the molecular weight of unknown organic compounds using Rast's micro method.	K3& K4
CO2	determine the strength of unknown solution potentiometrically.	K3& K4
CO3	estimate the concentration of unknown mixtures.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	M	S	S	M	M		M	S	S	M	M
CO2	M	S	S	M	M		M	S	S	M	M
CO3	M	S	S	M	M		M	S	S	M	M

S-Strong, M-Medium, L-Low

Non–Electrical experiments:

1. Heat of solution from solubility.
2. Heat of solution by calorimetry.
3. Molecular weight determination by Rast method using digital Beckmann thermometer.
4. Determination of activity and activity co–efficient by freezing point method.
5. Distribution coefficient and determination of equilibrium constant.
6. Thermal analysis of simple binary systems.

Electrical experiments

1. Determination of pH and pKa values using quinhydrone and glass electrodes; Potentiometric titrations. (Acid–base, redox and precipitation).
2. Determination of solubility of sparingly soluble salt by EMF method.
3. Determination of activity coefficients from EMF data.

References

1. S.R. Palit and S.K. De, Practical Physical Chemistry Science Book Agency, Calcutta.
2. P.C. Sharma and Agarwal, Goel Publishing House, Meerut.
3. V. Venkateswaran, R. Veeraswamy and A. R. Kulaindaivelu, Practical Physical Chemistry, S. Chand & Sons.
4. J. B. Yadav, Advanced Physical Practical Chemistry, Goel Publications.

Course Title	**:**	**Core: Physical Chemistry-II (Thermodynamics)**	**Course Code**	**:**	**20PCH3C07**
Year	**:**	**II**	**Semester**	**:**	**III**
Hours/Week	**:**	**5**	**Credit**	**:**	**5**

Course Objectives:

Enable the students to

1. know the concept of fugacity, activity and chemical potential
2. acquire knowledge on third law of thermodynamics, probability and ensembles
3. gain knowledge about the distribution law (classical and statistical) and their applications
4. get knowledge on Maxwell-Boltzmann distribution law and its velocities
5. learn about Maxwell-Boltzmann, Fermi Dirac and Bose Einstein statistics
6. acquire knowledge about equipartition principle of energy

Course Outcomes

After learning the course, the students will be able to

CO1	apply the concept of fugacity, activity and chemical potential	K3& K4
CO2	explain the laws of thermodynamics and probability	K1 & K2
CO3	understand the Boltzmann distribution law and its various applications.	K2
CO4	analyse the classical and statistical thermodynamics and their applications.	K4
CO5	distinguish the concepts of Maxwell-Boltzmann, Fermi Dirac, Bose Einstein statics and equipartition principle of energy.	K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	S	S	M	M	L		S	S	M	M	L
CO3	S	S	M	M	L		S	S	M	M	L
CO4	S	S	M	M	L		S	S	M	M	L
CO5	S	S	M	M	L		S	S	M	M	L

S-Strong, M-Medium, L-Low

UNIT–I

Thermodynamics of non–ideal systems–concept of chemical potential, Gibbs–Duhem equation, variation of chemical potential with temperature and pressure.Concept of fugacity of gases, determination by graphical method and from equation of state.Variation of fugacity with temperature and pressure.Fugacity and standard state of non–ideal gases, fugacity coefficient.Definition of activity and activity coefficient.Variation of activity of gas with pressure and temperature.Standard states.Determination of solvent activity by vapour pressure method,

cryoscopic method, activity of one component from that of other component (Gibbs–Duhem equation), mean activities of electrolytes.Determination of activity of solute.

UNIT–II.

Probability: Definition and laws of probability. Thermodynamic probability.Boltzmann expression of entropy.Probability and the third law.Statistical meaning of the third law and apparentexceptions.Irreversible or non-equilibrium thermodynamics. Phenomenological laws and Onsager's reciprocal relations, linear phenomenological relations–conjugate flows. Entropy production–examples of entropy production, Prigogine's principle of minimum entropy production, entropy production in coupled phenomena, Seebeck effect, Peltier effect.

UNIT–III.

Maxwell's distribution law of molecular velocities in an ideal gas.Experimental verification of Maxwell's distribution law.Evaluation of average velocity, root mean square velocity and most probable velocity from distribution law.Maxwell's distribution of molecular energies.The principle of equipartition of energy and the calculation of heat capacities of ideal gases.Limitations of the principle of equipartition of energy. Maxwell–Boltzmann statistics. Stirling's approximation, Langrangian multipliers.Maxwell Boltzmann distribution law.Evaluation of alpha and beta in Maxwell–Boltzmann distribution law.Limitations of Maxwell–Boltzmann distribution law.

UNIT–IV.

Partition function: Definition, justification of nomenclature. Microcanonical and canonical ensembles. Molecular partition function and Canonical partition function. The relation between the total partition function of a molecule and the separate partition function.Translational partition function. Entropy of monoatomic gases, rotational partition function. Effect of molecular symmetry on rotational partition function.Ortho and para hydrogen.Vibrational partition function. Electronic partition function, Nuclear partition function. Evaluation of thermodynamic function E, H, S, G, Cv and Cp from partition functions. Calculation of equilibrium constants of reactions involving ideal gases from partition functions.

UNIT–V

Heat capacities of solids–Einstein and Debye theories of heat capacities of solids. Bose–Einstein and Fermi–Dirac statistics. Bose–Einstein distribution law. Plank distribution law for black–body radiation. (Bose–Einstein ideal photon gas) Bose–Einstein condensation. Fermi–Dirac Distribution law, ideal Fermi–Dirac gas–electron gas in metal–Fermi energy.

References

1. L.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, W.A.Benjamin (1974).
2. J.F. Lee, F.W. Sears and L. Turcotte, Statistical Thermodynamics, Addision–Welsley (1973).
3. M.C. Gupta, Statistical thermodynamics, New Age International (1990).
4. S. Glasstone, Thermodynamics for chemists, affiliated East West press (1964).
5. F.T. Wall, Chemical Thermodynamics, Freeman and Company (1965).
6. L.K. Nash Chemical Thermodynamics II, Addision Wesley Publishing (1976).
7. Gurdeep Raj Advanced Physical Chemistry, Goel Publishing House (2012).

E-resources:

1. https://freevideolectures.com/course/5030/nptel-thermodynamics
2. https://www.youtube.com/watch?v=JfJ7MlP9Dco
3. https://www.youtube.com/watch?v=pFVSue8SjGU
4. https://www.youtube.com/watch?v=5DfGACOKul4
5. https://www.youtube.com/watch?v=tZYsVKUjn9E

Course Title	**:**	**Core: Organic Chemistry-III** (Chemistry of Natural products)	**Course Code**	**:**	**20PCH3C08**
Year	**:**	**II**	**Semester**	**:**	**III**
Hours/Week	**:**	**5**	**Credit**	**:**	**5**

Course Objectives:

Enable the students to

1. know the methods of isolation, classification, and structural elucidation of important terpenoids.
2. know the structural elucidation and synthesis of cholesterol by chemical analysis.
3. learn the general methods of elucidation of structure of alkaloids, and synthesis of some important alkaloids.
4. imbibe knowledge on the synthesis of peptides, and structural elucidation of proteins in detail.
5. understand the chemistry of pigments and co-pigments.
6. study about importance of antibiotics and sulfa drugs as chemotherapeutic agents.

Course Outcomes

After learning the course, the students will be able to

CO1	describe the isolation, classification, structural elucidation and synthesis of important terpenoids, alkaloids and steroids.	K1& K1
CO2	understand the structural elucidation ,synthesis and biosynthesis of cholesterol, ergosterol through chemical analysis	K1&K2
CO3	discuss the general methods of structural elucidation and apply these methods to the structural elucidation of alkaloids.	K3& K4
CO4	explain synthesis , properties and biological functions of polypeptides and proteins. Analyse the structure of proteins.	K3& K4
CO5	demonstrate the chemotherapeutical activity of chemical compound and analyse their structure activity relationships and their applications.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	S	S	M	M	L		S	S	M	M	L
CO3	S	S	M	M	L		S	S	M	M	L
CO4	S	S	M	M	L		S	S	M	M	L
CO5	S	S	M	M	L		S	S	M	M	L

S-Strong, M-Medium, L-Low

UNIT–I

Terpenoids–Isolation, classification, isoprene rule and special isoprene rule. Structural elucidation and synthesis of zingiberene, β–eudesmol, caryophyllene and abietic acid and biosynthesis of terpenoids.

UNIT–II

Cholesterol–structural elucidation (synthesis not required)–conversion of cholesterol into testosterone and progesterone.Ergosterol–Structure–conversion into progesterone. Structural discussion of vitamin–D, testosterone and progesterone.Oestrone–Structure and Hughes *et al* synthesis–Equilenin–structure and synthesis.Biosynthesis of steroids.

UNIT–III

General methods of ascertaining structure of alkaloids. Structural elucidation and synthesis of quinine, morphine, codeine, thebaine, reserpine and brucine. Structure of cortisones.

UNIT–IV

Polypeptides–General principles of polypeptide synthesis, Bergmann and Sheehan *et al* methods and Solid state peptide synthesis. Proteins–characteristics, Classification, end group analysis, primary, secondary, tertiary and quaternary structures. Oxytocin–structure and synthesis. Enzymes and coenzymes, biosynthesis of proteins, Structures of RNA and DNA and their biological importance.

UNIT–V

Natural Plant Pigments and co–pigments: Anthocyanins–structure of anthocyanidins and synthesis. Flavones and isoflavones–structure and synthesis. Baker–Venkataraman synthesis and Kostanecki synthesis. Flavonol–structure and synthesis.

Chemotherapy : Penicillin–structural elucidation and synthesis. Sulpha drugs–prepartion and uses of sulpha pyridine, sulphathiazole and sulphaguanidine. Mode of action of sulpha drugs.

References

1. L.Finar, Organic chemistry Vol.I& II, ELBS LongmannGroup.(2011).
2. O.P. Agarwal, Natural Product Chemistry, Goel Publishing House(2001).
3. Gurdeep R. Chatwal, The Chemistry of Organic Natural Products Vol. I & II, Himalaya Publishing House (2009).

E-resources:

1. https://freevideolectures.com/course/3266/heterocyclic-chemistry
2. https://www.youtube.com/watch?v=h1Z1iwhbtBo
3. https://www.youtube.com/watch?v=OxQzr6tXYFQ
4. https://www.youtube.com/watch?v=oOya3cFmAMc
5. https://www.youtube.com/watch?v=oofh4pKfXl0

Course Title	**:**	**Core: Organic Reactions and Reagents**	**Course Code**	**:**	**20PCH3C09**
Year	**:**	**II**	**Semester**	**:**	**III**
Hours/Week	**:**	**5**	**Credit**	**:**	**5**

Course Objectives:

Enable the students to

1. enable the students to gain knowledge on molecular rearrangements and to differentiate them
2. understand the chemistry and importance various reagents and their applications in organic synthesis
3. identify the organic compounds using chemical reactions and elemental composition

Course Outcomes

After learning the course, the students will be able to

CO1	describe the molecular rearrangements and discuss the applications of naming reactions	K1& K2
CO2	elaborate the preparation and synthetic applications of some of the organometallic reagents	K2 & k3
CO3	explain the mechanism and applications of some of the organic named reactions.	K2 & k3
CO4	apply organic reagents to synthesis new organic compounds.	K3& K4
CO5	apply chemical reactions and elemental composition to identify the unknown organic compounds.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	M	S	M	L		S	S	M	M	L
CO2	S	M	S	M	L		S	M	M	M	L
CO3	S	S	M	M	L		S	S	S	M	L
CO4	M	S	S	M	M		M	S	S	M	S
CO5	M	S	S	M	S		M	S	S	M	S

S-Strong, M-Medium, L-Low

Unit–I

Molecular rearrangements–mechanism and applications of Wagner–Meerwein, Wolf, Sommelet–Hauser, Beckmann, Neber, Baeyer–Villiger oxidation, Dakin, Steven, Favorskii, Orton, Dienone–phenol, Benzidine, Fries and Photo Fries rearrangements.

Unit–II

Preparation and synthetic applications of organometallic compounds–Organolithium, Organozinc, Organocadmium, Organomercury, Organolead, OrganoaluminiumOrganoboranes compounds and Grignard reagents.

Unit–III

Mechanism and applications of Named reactions–Arndt–Eistert synthesis, Elbspersulphate oxidation, Leuckart, Pechmann, Reformatsky, Wittig, Sandmeyer, Ullmann, Gomberg, Willgerdot, Wurtz, Fittig andUmpolung reactions.

Unit–IV

Reagents in organic synthesis–Preparation and applications of NBS, Osmium tetroxide, ozone, periodic acid, $Pd/BaSO_4$, Selenium, Selenium dioxide, Sodium borohydride, Lead tetra acetate, DDQ, DCC, PPA, B_2H_6 and C_6H_5COOOH.

Unit–V

Problems in organic chemistry using basic chemical reactions and elemental composition–involving hydrocarbons, aromatic hydrocarbons, alkyl halides, alcohols, aryl halides, phenols, carbonyl compounds, carboxylic acids, esters, nitro compounds, amines, nitriles. (Spectral data should not be included)

Books for study and Reference

1. O. P. Agarwal, Reactions and Reagents, Goel Publishing House (2006).
2. S. N. Sanyal, Reactions, Rearrangements and reagents, Bharathi Bhawan Publishers (2008).
3. V. K. Ahluwalia and R. K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House (2002).
4. P. L. Soni and H. M. Chawala, Text Book of Organic Chemistry, Sultan Chand & Sons (2007).
5. Jagadamba Singh and L. D. S. Yadav, Advanced Organic Chemistry, PragatiPrakashan (2004).

E-resources:

1. https://www.youtube.com/watch?v=dnam2PHjuwQ
2. https://freevideolectures.com/course/2642/chemistry-51a-organic-chemistry
3. https://freevideolectures.com/course/4114/nptel-reagents-in-organic-synthesis
4. https://engineering.eckovation.com/30-important-name-reactions-organic-chemistry- iit-jee/
5. https://www.youtube.com/watch?v=mrOm_HKPqE0

Course Title	**:**	**Elective: Computational Chemistry And Molecular Modelling**	**Course Code**	**:**	**20PCH3EL3**
Year	**:**	**II**	**Semester**	**:**	**III**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. learn the principles of computational chemistry and computer-based molecular modelling in both molecular mechanical and quantum mechanical models.
2. impart knowledge in quantum chemistry, molecular mechanics, bioinformatics and theoretical characterization of molecules.
3. introduces the applied methods for computation of the geometric and electronic structure-function of molecules.

Course Outcomes

After learning the course, the students will be able to

CO1	distinguish between theoretical approaches such as Ab initio, DFT, semi-empirical and force field methods.	K1& K2
CO2	analyse variety of commonly used computational techniques, such as geometry optimization, location of transition states, conformational analysis, and apply them to predict the molecular and spectroscopic properties.	K2 K3 & K4
CO3	analyse the computational tools and apply the right computational tool in their field of research.	K3 & K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	S	S	M	M	L		S	S	M	M	L
CO3	S	S	M	M	L		S	S	M	M	L

S-Strong, M-Medium, L-Low

Unit I : Molecular Mechanics

Force fields and molecular representations of matter - potential energy functions, inter- and intra-molecular interactions, empirical parameters, constraints and restraints, united atom and coarse-grained approaches, non-pairwise interactions. Energy minimization techniques- steepest descent, conjugate gradient, Newton-Raphson, simulated annealing, branch-and-bound and simplex.

Unit II : Molecular Dynamics

Elementary concepts of Ensembles and fluctuations, non-bonded cutoffs, long-range interactions, periodic boundaries, partition function, ensemble averaging and ergodicity. Trajectory analysis - conformational analysis and normal mode analysis. Brownian dynamics, free energy perturbation methods and Monte Carlo simulation.

Unit III : Quantum Mechanics

Basis set: Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, correlation-consistent sets, core-valence sets, general contractions.

Semi-empirical method: π-methods, valence electron methods - extended Hückel, neglect of differential overlap methods - Austin Model 1, Parameter Model 3.

Ab initio theory: restricted and unrestricted Hartree-Fock, electron correlation, many body perturbation theory, coupled cluster theory and multi configuration self-consistent field theory.

Density functional theory: homogeneous electron gas, Coulomb hole, exchange hole, use of density functional theory in quantum chemistry, Kohn-Sham equations, exchange, correlation and hybrid functional.

QM/MM Method: Mixed methods like the combination of quantum chemical methods and molecular mechanics (QM/MM) for the description of biochemical problems with specific reference to the interaction between drug and receptor.

Unit IV : MM Modelling

MM Modelling I: Biomolecular structure modelling, visualization and database

MM Modelling II: Parameterization of force field

MM Modelling III: Ligand docking and binding pocket analysis

MM Modelling IV: Tool handling

MM Modelling V: Solvation modelling explicit *vs* implicit

MM Modelling VI: Energy minimization techniques and conformation analysis

MM Modelling VII: Molecular dynamics simulation and analysis

MM Modelling VIII: Monte Carlo simulation in chemical and biochemical applications

Unit V : QM Modelling

QM Modelling I: Electronic structure building

QM Modelling II: Basis Sets and Basis Set Superposition Error

QM Modelling III: Single point and geometry optimization calculation

QM Modelling IV: Atomic charges, dipole moment, polarizability and hyper polarizability

Electronic spin - $\hat{S}^2$ operator and degeneracy

Group theory - molecular point groups and term symbols

QM Modelling V: Vibrational frequency analysis, symmetry analysis, harmonic vs fundamental frequencies, zero-point vibrational energies, Hessian index and distinguishing minima from transition states

QM Modelling VI: Reaction profiles in gas phase reaction, solvent effects, thermodynamic properties and intrinsic reaction coordinates analysis

QM Modelling VII: Prediction of theoretical UV-vis, IR and NMR Spectroscopy

QM/MM Modelling VIII: Protein-Ligand interaction, modelling enzymatic reaction profile

References

1. F. Jensen, *Introduction to Computational Chemistry*, Wiley, New York, 1999.
2. Christopher J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2nd Ed. Wiley & Sons, New York, 2004.
3. Andrew R. Leach, *Molecular Modelling: Principles and Applications*, 2nd Ed., Prentice Hall, 2001.
4. David Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*, John Wiley & Sons, 2004.
5. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st Ed, Dover, 1989.

E-resources:

1. https://www.youtube.com/watch?v=najTlj2_lN8&list=PLOzRYVm0a65fCJJQendw
2. https://www.youtube.com/watch?v=najTlj2_lN8&list=PLOzRYVm0a65fCJJQendw EEcSrC8iwvgBn
3. https://www.youtube.com/watch?v=gP6HfBQ_LkI
4. https://www.youtube.com/watch?v=3uY5N3rgoLE
5. https://www.youtube.com/watch?v=0FBZFhwJgp8

Course Title	**:**	**Core: Physical Chemistry-III (Chemical Kinetics and Electrochemistry)**	**Course Code**	**:**	**20PCH4C10**
Year	**:**	**II**	**Semester**	**:**	**IV**
Hours/Week	**:**	**5**	**Credit**	**:**	**5**

Course Objectives:

Enable the students to

1. enrich the idea about the various types of reactions
2. supplement the various catalytic mechanisms
3. teach the concepts of electrical double layer
4. impart the applications of electro kinetic phenomena

Course Outcomes

After learning the course, the students will be able to

CO1	explain the theories of reaction rates and analyse the influence of solvent, ionic strength and pressure on reaction rate in solution.	K3& K4
CO2	distinguish the kinetics of various types of chemical reactions.	K2& K4
CO3	recognise characteristics of various types of catalytic reactions and its applications	K1 & K2
CO4	describe the electrochemical principles of corrosion, classification and prevention of corrosion process.	K1& K2
CO5	demonstrate theprinciple, working and applications of electro analytical techniques.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	L	M		S	S	M	L	M
CO2	S	S	M	M	L		S	S	M	M	L
CO3	S	S	M	L	M		S	S	M	L	M
CO4	S	S	M	M	L		S	S	M	M	L
CO5	M	S	S	M	S		M	S	S	M	S

S-Strong, M-Medium, L-Low

UNIT–I

Theories of reaction rates: Hard sphere collision theory of gas–phase reaction, potential energy surfaces, absolute reaction rate theory–formulation in terms of partition function, relation between activated complex theory and hard sphere collision theory, thermodynamic formulation of activated complex theory (ARRT). Kinetic isotopic effects. Reactions in solution–comparison between gas–phase and solution reactions, cage effects. The influence of solvent on the reactions between ions and neutral molecules. Influence of ionic strength on rates of reactions in solution. Primary and secondary salt effects. Influence of pressure on rates of reactions in solution.

UNIT–II

Kinetic treatment of complex reactions: Parallel reactions of the same order (first and second order), reversible reactions of the same order (first), first order forward and second backward, consecutive first order reactions. Steady state approximation, chain reactions and explosions. Fast reaction–definition–study of fast reactions–flow method, pulse method, relaxation method, shock–tube method, nuclear magnetic resonance method.

UNIT–III

Homogeneous catalysis**:** Specific and general acid–base catalysis, Bronsted catalysis law. Acidity functions–definition–significance, enzyme catalysis (single substrate reaction only), Michaels–Menten Kinetics, influence of pH and temperature on enzyme catalysis. Surface phenomenon–physisorption and chemisorption. Adsorption isotherms: Freundlich, Gibbs, Langmuir and BET. Kinetics and mechanism of heterogeneous catalysis(Langmuir–Hinshelwood and Langmuir–Rideal–Eley).

UNIT–IV

Activity, activity coefficient, ionic strength–Debye–Huckel limiting law. Dynamic electrochemical process at electrodes–electrical double layer–Helmholtz, Gouy–Chapman and Stern models. Corrosion–classification of corrosion processes, conditions for the occurrence of corrosion processes, electrochemical principles of corrosion, prevention of corrosion.

UNIT–V

Electrokinetic phenomena: Electrolytic oxidation and reduction. Voltametry and polorography–current–voltage relationships. Migration current,diffution current, residual current, half–wave potential. Ilkovic equation, dropping mercury electrode, applications of polarography. Amperometrictitrations.Fundamental principles of coulometry–constant current and controlled potential methods–primary and secondary titrations.

References

1. K.J. Laidler, Chemical kinetics, Harper and Row publication (1965).
2. W.J. Moore, Physical Chemistry, Longmann's (1975).
3. S. Glasstone, An Introduction to Electrochemistry, affiliated East–West press(2004).
4. L.L. Andropov, Theoretical electrochemistry, Mir Publishers (1972).
5. Raj Narayan, An Introduction to Metallic Corrosion and its Prevention, Oxford and IBH Publishing Co(1983).
6. P.W. Atkins, Physical Chemistry VIEdition, Oxford University (1998).
7. Gurudeep Raj, Advanced Physical Chemistry, Goel Publishing House. (2012).

E-resources:

1. https://www.khanacademy.org/science/chemistry/chem-kinetics#reaction-rates
2. https://freevideolectures.com/course/3326/heterogeneous-catalysis-and-catalytic-processes
3. https://freevideolectures.com/course/4594/nptel-bioelectrochemistry/1
4. https://www.youtube.com/watch?v=LDcYwgSsNyw
5. https://www.youtube.com/watch?v=3olOk_xNq8g

Course Title	**:**	**Elective: Nano Science and Green Chemistry**	**Course Code**	**:**	**20PCH4EL4**
Year	**:**	**II**	**Semester**	**:**	**IV**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. enable the students to understand the basic principles and importance of nano and green chemistry
2. acquire knowledge on various of synthetic methods, properties and applications of nanomaterials
3. study microwave and ultra sound assisted synthesis of organic compounds and nanomaterials
4. understand the concept of ionic liquids and phase-transfer catalysis with their applications
5. apply the green chemistry ideas for cleaner environment

Course Outcomes

After learning the course, the students will be able to

CO1	describe the basic concepts, synthetic methods and applications of nano materials.	K1 & K2
CO2	analyse the characteristic properties of nano materials through various instrumentation techniques and understand the properties and applications of nanomaterials.	K2& K4
CO3	explain the basic concepts of green chemistry and green reactions. analyse the characteristics of green chemical reactions.	K2 & K4
CO4	understand the characteristics of green solvents and phase transfer catalyst and analyse the reactions carried out in green solvents.	K3& K4
CO5	employ the green chemical compounds, reagents and solvents forclean environment.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	S	S	M	M	L		S	S	M	M	L
CO3	S	S	M	M	M		S	S	M	M	M
CO4	S	S	M	M	M		S	S	M	M	M
CO5	S	S	M	L	M		S	S	M	M	M

S-Strong, M-Medium, L-Low

UNIT I

Introduction to nanotechnology: Basic ideas and terminology. Classification based on dimension. Various nanostructures: Nanowires, nanorods, nanoballs, nanotubes and nanofluids. Fullerenes and graphenes (basic ideas only). Synthetic techniques of nanomaterials: Top down and bottom up approaches-lithography. Physical methods: Laser ablation, evaporation and sputtering. Chemical

methods: sol-gel synthesis, co-precipitation, microwave and sonochemical methods. Synthesis and uses of certain nanoparticles: Gold, silver, zinc oxide, iron oxide and TiO_2.

UNIT –II

Characterisation of nanomaterials by UV, Fluorescence, X-Ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Atomic force microscopy (AFM) and Scanning tunnelling electron microscopy (STEM). Properties of nanoparticles:Optical properties, magnetic properties-diamagnetic, paramagnetic, ferromagnetic and super paramagnetic properties. Size dependent properties-coercivity and saturation magnetization. Applications of nanoparticles in the fields of medicine, energy sector, catalysis, water purification and automobiles. Nanopollution- safety and ethics.

UNIT III

Introduction of Green Chemistry-Twelve principles of green chemistry and atom economy calculations. Microwave assisted synthesis: Microwave heating, advantages of microwave exposure. Organic synthesis in water: Hofmann elimination, hydrolysis of benzyl chloride, hydrolysis of methyl benzoate. Organic synthesis in organic solvents: Esterification and synthesis of chalcone. Solvent free synthesis-Fries rearrangement. Ultrasound assisted reactions: Homogeneous reactions: Curtius rearrangement, annulations and Diels-Alder reaction. Heterogeneous reactions: Esterification, saponification and reduction.

UNIT IV

Organic synthesis in benign green solvents: Water- Pinacol coupling, Claisen rearrangement, Wittig-Horner reaction, Heck reaction and Strecker synthesis. Super critical carbon dioxide:Properties and its applications in asymmetric synthesis, polymerization, Freidel-Crafts reaction and hydrogenation.Ionic liquids: Types, preparation and properties. Task specific ionic liquids- Bronsted acidic and basic ionic liquids. Use of ionic liquids in the synthesis of cyclic carbonates, 1-acetylnaphthalene and epoxides. Organic synthesis using phase transfer catalysts (PTC): Mechanism, types and advantages of PTC. Applications of PTC in the synthesis of Benzoin and flavones.

UNIT V

Applications of Green Chemistry for Cleaner environment:Super critical carbon dioxide in dry cleaning, as a cleaning solvent in the manufacture of ICs and computer chips. Biodegradable polymer from renewable sources - polylactic acid. Closed loop recycling of PET. Thermal polyaspartate as antiscalant. H_2O_2-eco friendly bleaching agent in paper industry. Yttrium oxide-eco-friendly corrosion inhibitor.TiO_2- as green photo catalyst for destroying hazardous pollutants.

Books for Reference

1. Environmental Chemistry with Green Chemistry, Ashim. K. Das and Madhua. Das, Books and Allied Pvt. Ltd. (2012)
2. Green Chemistry A Text Book V. K. Ahluwalia, Narora Publishing House.(2013)

3. Green Chemistry-Greener Alternatives to synthetic alternatives to synthetic organic transformations,V. K. Ahluwalia, Narora Publishing House. (2011)
4. A Text Book of Nano Science and Nano Technology, T. Pradeep Tata McGraw Hill Publishing Company Ltd. (2012).
5. Nano Technology, S. Shanmugam, MJP Publishers .(2012)
6. Text Book of Nano Science and Nano Technology, R. S. Murthy, P. Shankar, Baldev Raj, B. B. Rath and James Murday, University Press (2012)
7. Introduction to Nano Science and Nano Technology, K. K. Chattopadhyay and A. N. Banerjee, PHI Learning Pvt Ltd (2012)

E-resources:

1. https://www.youtube.com/watch?v=0MzIh7wkgMs
2. https://www.youtube.com/watch?v=lFYs3XDu4fQ
3. https://www.youtube.com/watch?v=J9SpYVx8H68
4. https://www.youtube.com/watch?v=uYit6N-lIEI
5. https://www.youtube.com/watch?v=Kthhnd5kmDo

Course Title	**:**	**Elective: Medicinal Chemistry**	**Course Code**	**:**	**20PCH4EL5**
Year	**:**	**II**	**Semester**	**:**	**IV**
Hours/Week	**:**	**5**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. recognise the basic concepts about drugs designing and structure activity relationships QSAR etc.
2. know about the various types ofanaesthetics and its chemistry.
3. acquire the knowledge about sedative, hypnotics, analgesics and antibiotics. Their mode of action and synthesis.

Course Outcomes

After learning the course, the students will be able to

CO1	explain the basic concepts of drug and understand the drug designing and factors governing it.	K1& K2
CO2	discuss the characteristics of anaesthetics, synthesis and classification.	K2
CO3	describe the synthesis and characteristics of sedatives and hypnotics	K2
CO4	elaborate the mode of action and synthesis of CNS stimulants.	K2 & K4
CO5	explain the mode of action, structure activity relationship and synthesis of antibiotics and cardiovascular drugs.	K2 & K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	S	S	M	M	L		S	S	M	M	L
CO2	S	S	M	M	L		S	S	M	M	L
CO3	S	S	M	M	L		S	S	M	M	L
CO4	S	S	M	M	L		S	S	M	M	L
CO5	S	S	M	M	L		S	S	M	M	L

S-Strong, M-Medium, L-Low

UNIT I

Introduction to drugs: requirements of ideal drugs, sources and classification. Drug design – aim and factors governing drug design. Adsorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) and Quantitative Structure Activity Relationship (QSAR). Clark and Paton's theory.

UNIT II

Anaesthetics – requirements of anaesthetics – classification. General anesthetics – classification and mode of action. Inhalation anaesthetics - synthesis, advantages and disadvantages of ether and chloroform. Intravenous anaesthetics – synthesis of thiopental sodium and ketamine hydrochloride.

Local anaesthetics – requirements, classification, synthesis of benzocaine and dimethisoquin.

UNIT III

Sedatives and Hypnotics – synthesis of phenobarbitone and paraldehyde. Anticonvulsants – synthesis of phenytoin sodium and troxidone - mode of action of anticonvulsants. Gastrointestinal agents – antacids – synthesis of magnesium carbonate, aluminium hydroxide gel and magnesium trisilicate.

UNIT IV

Central nervous system (CNS) stimulants – mode of action, synthesis of caffeine and nikethamide.

Antipyretic analgesics – mode of action, synthesis and uses of paracetamol, aspirin and salol.

Expectorants and antitussives – synthesis of acetylcysteine, guaifensin and benzonatate.

Disinfectants and antiseptics – distinction and types.

UNIT V

Antibiotics – requirements of antibiotics – classification. Penicillin, chloramphenicol, tetracyclines and streptomycin - structure activity relationship.

Cardiovascular drugs – mode of action. Synthesis of diazoxide and clonidine.

Introduction to anti- HIV and anti- cancer drugs.

References

1. AshutoshKar, Medicinal Chemistry, New Age international Publishers, New Delhi, Edn .2
2. G.R. Chatwal Pharmaceutical Chemistry, Organic Volume II, Himalaya Publishing House, New Delhi.
3. Graham. L. Patrick, An introduction to Medicinal Chemistry, Oxford University Press Edn. 3.

E-resources:

https://freevideolectures.com/course/4198/nptel-medicinal-chemistry

2. https://www.youtube.com/watch?v=hEUj-ZcxkcM
3. https://www.youtube.com/watch?v=xGX_fvSmzI0
4. https://www.youtube.com/watch?v=b7iR8pgOEYs
5. https://www.youtube.com/watch?v=4mc-g-m_wSA

Course Title	**:**	**Core Practical: Inorganic Chemistry-II**	**Course Code**	**:**	**20PCH4CP4**
Year	**:**	**II**	**Semester**	**:**	**III &IV**
Hours/Week	**:**	**3**	**Credit**	**:**	**3**

Course Objectives:

Enable the students to

1. learn the estimation of ions using EDTA by complexometic titration.
2. know the setup of various chromatographic techniques and their applications.
3. give an idea about the preparation of inorganic complexes.
4. inculcate about the estimation of metal ions from the given mixture by using volumetric as well as gravimetric methods.

Course Outcomes

After Learning the Course, the students will be able to

CO1	estimate the amount of ions and also hardness of water using complexometric titrations.	K3& K4
CO2	demonstrate the various chromatographic technique setup and understand their applications.	K2
CO3	estimate the mixture of cations using volumetric and gravimetric analyses.	K3& K4
CO4	prepare the inorganic complexes.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	M	S	S	M	S		M	S	S	M	S
CO2	M	S	S	M	M		M	S	S	M	M
CO3	M	S	S	M	S		M	S	S	M	S
CO4	M	S	S	M	S		M	S	S	M	S

S-Strong, M-Medium, L-Low

1. Titrimetry: oxidation using ceric salts; complexometric titration involving estimation of calcium, magnesium, nickel, zinc and hardness of water using EDTA.

2. Chromatography: Column, Paper, thin layer and ion exchange. (Demonstration)

3. Preparation of the following inorganic complexes: Pentathioureadicuprous nitrate, Potassiumtrioxalatoferrate(III),trans–Potassiumdiaqua(dioxalato)chromate(III), Hexaamminecobalt (III) chloride and Ammoniumhexachlorostannate(IV).

4. Quantitative estimation:

Mixture of cations involving volumetric and gravimetric estimation:

Copper and nickel, copper and zinc, copper and magnesium, iron and nickel, iron andmagnesium and calcium and barium.

References

1. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, Principles of Practical Chemistry, Sultan Chand & Sons.
2. S. Giri. D. N. Bajpai and O. P. Panday, Practical Chemistry Vol. I & II S.Chand& Company
3. J. Bassart, R. C. Dennay, G. H. Jeffery and Mendham, Vogels text book of qualitative Inorganic analysis, The ELBS & Longman.

Course Title	**:**	**Core Practical: Organic Chemistry-II**	**Course Code**	**:**	**20PCH4CP5**
Year	**:**	**II**	**Semester**	**:**	**III &IV**
Hours/Week	**:**	**3**	**Credit**	**:**	**3**

Course Objectives:

Enable the students to

1. learn the chemistry involved in quantitative estimation of organic compounds
2. understand the chemistry behind the qualitative analyses of oil.
3. know the chemical methods of extraction of active constituents
4. Recognise the chemistry involved in preparation of organic compounds

Course Outcomes

After learning the course, the students will be able to

CO1	estimate the amount of organic compounds	K3& K4
CO2	analyse the oils qualitatively	K3& K4
CO3	extract the active constituents from the various sources.	K3& K4
CO4	prepare various organic compounds.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	M	S	S	M	S		M	S	S	M	S
CO2	M	S	S	M	S		M	S	S	M	S
CO3	M	S	S	M	S		M	S	S	M	S
CO4	M	S	S	M	S		M	S	S	M	S

S-Strong, M-Medium, L-Low

1. Quantitative Estimation:

Phenol, aniline, acetone, glucose (Bertrand's and Fehling's methods) nitro, amino and methoxy group, and unsaturation.

2. Analysis of Oil (Reichart–Meisel value, Iodine value, Saponification value and acetyl value)

3. Extraction and estimation of active constituents: (Group experiment)

a) Lactose from milk
b) Caffeine from tea leaves.
c) Nicotine from Tobacco extract.
d) Citric acid or ascorbic acid from a tablet or from a natural source.

4. Preparations: At least five two stage preparations from literature.

References

1. B.B. Day, M.V. Sitaram and T.R. Govindachari, Laboratory Manual of Organic Chemistry, Allied Publishers Limited.
2. Gnanprakasam and Ramamurthy, Organic Chemistry Laboratory Manual, Ananda Book Depot, Chennai.
3. Jagmohan, Advanced Practical Organic Chemistry Vol. I & II.

Course Title	**:**	**Core Practical: Physical Chemistry-II**	**Course Code**	**:**	**20PCH4CP6**
Year	**:**	**II**	**Semester**	**:**	**III &IV**
Hours/Week	**:**	**4**	**Credit**	**:**	**4**

Course Objectives:

Enable the students to

1. enable the students to understand the principle of conductivity experiments and carry out conductometric titrations, verification of Ostwald dilution and Debye –HuckelOnsagar law
2. study the determination the rate constant for acid, base catalysed hydrolysis of esters
3. study the effect of temperature on rate constant and evaluation of Ea
4. acquire knowledge on the kinetics of adsorption of oxalic acid, acetic acid on charcoal and fitting into Freundlich–isotherm

Course Outcomes

After learning the course, the students will be able to

CO1	estimate the strength of the unknown solutions by conductivity method and verify Ostwald dilution and Debye –HuckelOnsagar law.	K3& K4
CO2	experiment and calculate the rate constant for ester hydrolysis and Ea.	K3& K4
CO3	apply Freundlich isotherm to study the nature of adsorption of oxalic acid on charcoal.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	M	S	S	M	S		M	S	S	M	S
CO2	M	S	S	M	S		M	S	S	M	S
CO3	M	S	S	M	S		M	S	S	M	S

S-Strong, M-Medium, L-Low

A. Electrical experiments:

1. Determination of

   i. Equivalent conductance of a strong electrolyte and verification of Debye–HuckelOnsagar law

   ii. Verification of Ostwald dilution law and determination of molar conductance at infinite dilution of weak electrolyte using Kohlrausch's law.

2. Conductometric determination of pKa of a weak acid.

3. Determination of the solubility of a sparingly soluble salt.

4. Conductometric titrations:

   i. Acid-Base Titration–Determination of the strength of strong acid, weak acid and mixture of acids.

   ii. Precipitation titration–Determination of the strength of KCl,KI and KCl and KI in the mixture.

B. Non–Electrical equipments

1. i. Determination of the strength of the acids from the ratio of rate constants, for the hydrolysis of an ester

   ii. Evaluation of Arrhenius parameters using acid hydrolysis of an ester.

   iii. Base catalysed hydrolysis of an ester.

2. Rate of reaction between persulphate and iodide ions, study of salt effects over the persulphate iodide reaction.

3. Evaluation of catalytic constant of strong acids for the iodination of acetone or hydrolysis of an ester.

4. Adsorption Experiments: Adsorption of oxalic and acetic acid on activated charcoal–

Freundlich–isotherm.

References

1. S. R. Palit and S. K. De, Practical Physical Chemistry Science Book Agency, Calcutta.
2. P. C. Sharma and Agarwal, Practical Physical Chemistry, Goel Publishing House, Meerut.

Course Title	**:**	**CORE: Project Work**	**Course Code**	**:**	**20PCH4CPR**
Year	**:**	**II**	**Semester**	**:**	**IV**
Hours/Week	**:**	**5**	**Credit**	**:**	**5**

Course Objectives:

Enable the students to

1. understand the importance of experimental analysis, scientific approach in solving problems of chemistry
2. educate and train the students to write scientific reports.

Course Outcomes

After learning the course, the students will be able to

CO1	identify a research problem and plan suitable research strategy and design the experimental setup for the problem,	K3& K4
CO2	interpret the experimental data, analyse the result and based on the experimental data provide solution for the problem.	K3& K4
CO3	apply theproblem-solving skill, demonstrative skill, analytical skill.	K3& K4

K1- Remember, K2- Understand, K3- Apply, K4- Analyse

CO/ PSO	PO1	PO2	PO3	PO4	PO5		PSO1	PSO2	PSO3	PSO4	PSO5
CO1	M	S	S	M	S		M	S	S	M	S
CO2	M	S	S	M	S		M	S	S	M	S
CO3	M	S	S	M	S		M	S	S	M	S

S-Strong, M-Medium, L-Low