AUXILIUM COLLEGE (AUTONOMOUS)

VELLORE

M.Sc. CHEMISTRY

Curriculum Development – National Needs

SEMESTER I

PCCHA20 - STEREOCHEMISTRY AND CONFORMATIONAL ANALYSIS

Year: I **SEM:** I	**Course Code** PCCHA20	**Title of the Course** Stereochemistry and Conformational Analysis	**Course Type** Theory	**Course Category** Core	**H/W** 5	**Credits** 5	**Marks** 100

Learning Objectives:

- To learn the concepts of stereochemistry, conformational analysis and their application in the determination of reaction mechanism.
- To understand the mechanism and stereo chemistry of substitution and elimination reactions.
- To gain knowledge about the optical rotatory dispersion and circular dichroism.

Course Outcomes:

The Learners will be able to

1. Assign the configuration of stereoisomers including those with no stereogenic carbon centre and classify the stereospecific and stereoselective reactions.
2. Compare the relative stability and reactivity of conformational isomers of cyclohexane and related compounds.
3. Ascertain the knowledge on the mechanism and stereo chemical outcome of aliphatic nucleophilic substitution reactions.
4. Compare the mechanistic spectra of elimination reactions.
5. Employ the principles of Optical Rotatory Dispersion and Circular Dichroism for various applications.

CO	**PSO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	M	H	M	H	H
CO2	H	M	H	M	H	H
CO3	H	M	M	H	H	H
CO4	H	M	M	H	H	H
CO5	H	H	H	H	H	H

CO	**PO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	M	M

CO2	H	H	H	H	M	M
CO3	H	H	H	H	M	M
CO4	H	H	H	H	M	M
CO5	H	H	H	H	M	M

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Chirality and optical activity - symmetry elements, classification of chiral molecules as asymmetric and dissymmetric. (K1, K2, K3, K4, K5 & K6)

1.2 Projection formulae - Sawhorse, Newmann and Fischer projections and their inter conversions. (K1, K2, K3, K4, K5 & K6)

1.3 Nomenclature - absolute configuration - R/S and D/L, relative configurations - threo/erythro and syn/anti. (K1, K2, K3, K4, K5 & K6)

1.4 A brief study of dissymmetry of allenes, biphenyls - atropisomerism, spiro compounds, transcyclooctene, cyclononene and molecules with helical structures. (K1, K2, K3, K4, K5 & K6)

1.5 Stereo specific and stereo selective reactions - definition and examples. Asymmetric synthesis - Cram's rule. (K1, K2, K3, K4, K5 & K6)

1.6 Geometrical isomerism - E/Z nomenclature of olefins, geometrical and optical isomerism of disubstituted cyclopropane, cyclobutane and cyclopentanes. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Conformational analysis of di-substituted cyclohexanes and their stereo chemical features - geometric and optical isomerism of these derivatives. (K1, K2, K3, K4 & K5)

2.2 Conformation and reactivity of cyclohexene - allylic 1, 2 and 1, 3 strains and related compound alkyldiene cyclohexane. (K1, K2, K3, K4 & K5)

2.3 Conformation of cyclohexanone - 2-alkyl and 3-alkyl ketone effect and reactivity of cyclohexanone in comparison with cyclopentanones. (K1, K2, K3, K4 & K5)

2.4 Conformations of six membered rings containing hetero atoms. (K1, K2, K3, K4 & K5)

2.5 Conformation and stereochemistry of cis and trans decalin and 9-methyl decalin. (K1, K2, K3, K4 & K5)

2.6 Quantitative correlation between conformation and reactivity - Curtin-Hammett principle. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 S_N2 reaction - kinetics, mechanism and factors influencing the reaction. (K1, K2, K3, K4, K5 & K6)

3.2 S_N1 reaction - kinetics, mechanism, factors influencing the reactions, rearrangement reaction. (K1, K2, K3, K4, K5 & K6)

3.3 Mixed S_N1 and S_N2 reactions - competition between S_N1 and S_N2 mechanism. (K1, K2, K3, K4, K5 & K6)

3.4 Substitution by ambident nucleophiles, substitution at allylic, vinylic, benzylic and aryl halides. (K1, K2, K3, K4, K5 & K6)

3.5 SET (single electron transfer) - types of electron transfer reactions - photo induced and chemically induced electron transfer. (K1, K2, K3, K4, K5 & K6)

3.6 Neighbouring group participation - introduction of an acyclic open chain system, Π systems of aromatic rings, cyclic system, double bond and σ bond. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 E_1, E_2, E_1CB reaction - kinetics, mechanism and evidences. (K1, K2, K3, K4 & K5)

4.2 E_1, E_2 and E_1CB variables - mechanistic spectrum, competition between elimination and substitution. (K1, K2, K3, K4 & K5)

4.3 Stereochemistry of E_2 - syn and anti-elimination reactions, orientation of the double bond. (K1, K2, K3, K4 & K5)

4.4 Regiochemistry of E_1, E_2 and E_1CB reactions with examples. (K1, K2, K3, K4 & K5)

4.5 Pyrolytic eliminations - acyclic and alicyclic systems, molecular rearrangements during elimination. (K1, K2, K3, K4 & K5)

4.6 Grob's fragmentations - incorporation of fragmentation - mechanism of fragmentation - mechanism allied to E_1 and E_2 eliminations. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Optical Rotatory Dispersion and Circular Dichroism - terminology - optical rotation, circular birefringence, circular dichroism and Cotton effect. (K1, K2, K3, K4, K5 & K6)

5.2 Plain curves - application of plain curves - determination of structure, configuration, conformation and optical activity. (K1, K2, K3, K4K5 & K6)

5.3 Rotatory dispersion of ketones - structure, configuration, conformation of unsaturated ketones. (K1, K2, K3, K4, K5 & K6)

5.4 Empirical and semi empirical rules - the axial halo ketone rule, the octant rule (configuration and conformation) (K1, K2, K3, K4, K5 & K6)

5.5 Absolute configuration and ketal formation. (K1, K2, K3, K4, K5 & K6)

5.6 Stereochemical analysis - polarimetry, chiral GC & HPLC and NMR techniques. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. R. O. C. Norman & Coxon, Principles of Organic Chemistry, NY, 3rd Edition, 2017.
2. S. M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry, MacMillan India Ltd., Chennai, Reprint 2010.
3. Stanley H Pines, Organic Chemistry, McGraw Hill Publication, 5th Edition, Reprint 2007.
4. Francis A. Carey and Richard J. Sundberg, Part A and B, Advanced Organic Chemistry, Plenum Press, 4th Edition, Reprint 2013.
5. Jerry March, Advanced Organic Reaction Mechanism and Structure, A Wiley Inter Science, 4th Edition, Reprint 2005.
6. D. Nasipuri, Stereochemistry of Organic Compounds, New Age Publishers, 2nd Edition, Reprint 2013.
7. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, New Age International Ltd, Reprint 2017.

8. Ernest L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill Publishing, Reprint 2007.
9. C. K. Ingold, Structure and Mechanism in Organic Chemistry, CBS Publishers and Distributors Pvt. Ltd., 2nd Edition, Reprint 2000.
10. P. S. Kalsi, Stereochemistry and Mechanism through Solved Problems, New Age International Publishers, Reprint 2003.
11. R. K. Bansal, Organic Reaction Mechanism, Tata McGraw Hill Publishing, 4th Edition, Reprint 2013.
12. Bernard Miller Advanced Organic Chemistry Reaction & Mechanism, Pearson Education, 2nd Edition, Reprint 2005.
13. P. S. Kalsi, Organic Reactions and their Mechanism, New Age International Publishers, 2nd Edition, Reprint 2017.
14. Nimai Tewari, Advanced Organic Stereochemistry (Problems & Solutions), Books and Allied (P), 1st Edition, 2010.

Open Educational Resources (OER):

1. https://babel.hathitrust.org/cgi/pt?id=umn.31951p01139217c&view=2up&seq=300
2. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-01, P-05)
3. https://www.hippocampus.org/HippoCampus/Chemistry;jsessionid=D178EB9CB8034395C03D09EFC98A06CA
4. http://ocw.uci.edu/lectures/chem_51a_lecture_13_organic_chemistry_ch_4_conformations_of_cyclohexane.html

SEMESTER I

PCCHB20 - STRUCTURAL INORGANIC CHEMISTRY

Year: I **SEM:** I	**Course Code** PCCHB20	**Title of the Course** Structural Inorganic Chemistry	**Course Type** Theory	**Course Category** Core	**H/W** 5	**Credits** 4	**Marks** 100

Learning Objectives:

- To learn the concepts of Lewis acids and bases.
- To learn the structures of complex solids, metals, and alloys.
- To gain knowledge about the structure and bonding in poly acids, boron hydrides and metal clusters.

Course Outcomes:

The Learners will be able to

1. Summarize the theories of acids and bases.
2. Discuss conductors, semiconductors and insulators based on band theory.
3. Assess the structure and bonding in different types of ionic solids, metals and alloys.
4. Discuss the structure and bonding in polyacids, silicates and inorganic polymers.
5. Distinguish the structure and bonding in boranes, carboranes, metallo carboranes, boron nitrides and metal clusters.

CO	**PSO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	M	M	H	H	H
CO2	H	M	M	H	H	H
CO3	H	M	M	H	H	H
CO4	H	M	M	H	H	H
CO5	H	M	M	H	H	H

CO	**PO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H

CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Acids and bases, proton transfer equilibria in water - solvent leveling effects. (K1, K2, K3, K4, K5 & K6)

1.2 Aqua acids - periodic trends in aqua acids - simple oxo acids - anhydrous oxides - polyoxo compound formation. (K1, K2, K3, K4, K5 & K6)

1.3 Lewis acid - base concepts, hard and soft acids and bases, group characteristics of Lewis acids. (K1, K2, K3, K4, K5 & K6)

1.4 Lux - Flood theory of acids and bases, Usanovich acids and bases, super acids and super bases. (K1, K2, K3, K4, K5 & K6)

1.5 Non aqueous solvents, classification, protic and aprotic solvents, molten salts as solvents and ionic liquids. (K1, K2, K3, K4, K5 & K6)

1.6 Heterogeneous acids and bases - symbiosis and proton sponges. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Structure of complex solids - layered structures - conducting ionic solids – graphite - solids held together by covalent bonding - diamond - Madelung constants. (K1, K2, K3, K4 & K5)

2.2 Imperfections in crystals - stoichiometric defects - Schottky, controlled valency, F-center and Frenkel defect - non-stoichiometric defects - metal excess defect, metal deficient defect - impurity defect. (K1, K2, K3, K4 & K5)

2.3 Band theory of solids, intrinsic and extrinsic semiconductors, piezoelectric and pyroelectric crystals. (K1, K2, K3, K4 & K5)

2.4 Superconductivity – Meissner effect, critical temperature and critical magnetic field - BCS theory. (K1, K2, K3, K4 & K5)

2.5 Type I and Type II superconductors. (K1, K2, K3, K4 & K5)

2.6 Ternary oxides - structures of 123 oxides (YBa-Cu- O) - applications of high temperature superconducting materials. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Structures of simple solids - unit cell and crystal structures. (K1, K2, K3, K4, K5 & K6)

3.2 Close packing of spheres - holes in closed packed structures. (K1, K2, K3, K4, K5 & K6)

3.3 Structure of metals and alloys - non-closed packed structures. (K1, K2, K3, K4, K5 & K6)

3.4 Atomic radii of metals - polytypism - polymorphism of metals. (K1, K2, K3, K4, K5 & K6)

3.5 Alloys - substitutional solid solutions, interstitial solid solutions of non-metals - intermetallic compounds. (K1, K2, K3, K4, K5 & K6)

3.6 Characteristic structures of ionic solids - binary phases (AX and AX_2) - ternary phases (ABO_3 and AB_2O_4). (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Structure and bonding - polyacids - isopolyacids and heteropolyacids of molybdenum and tungsten. (K1, K2, K3, K4 & K5)

4.2 Dawson and Keggins structure of poly acids, heteropolyanions and heteropoly blues. (K1, K2, K3, K4 & K5)

4.3 Inorganic polymers - silicates, structures, properties, correlation and applications. (K1, K2, K3, K4 & K5)

4.4 Molecular sieves, feldspar, zeolites and ultramarines and their applications. (K1, K2, K3, K4 & K5)

4.5 Polysulphur-nitrogen compounds - structure and bonding in tetrasulphur tetranitride, poythiazyl and S_xS_y compounds. (K1, K2, K3, K4 & K5)

4.6 Poly organo phosphazenes. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Structure and bonding - boron hydrides - introduction, classification of boranes - diborane, tetra borane, pentaborane, hexaborane and decaborane. (K1, K2, K3, K4, K5 & K6)

5.2 Polyhedral boranes - Wade's rule - closo, nido and arachno structures, hydroboration. (K1, K2, K3, K4, K5 & K6)

5.3 Carboranes - closo, nido and arachno structures of carboranes. (K1, K2, K3, K4, K5 & K6)

5.4 Metallocarboranes - closo, nido and arachno structures of carboranes. (K1, K2, K3, K4, K5 & K6)

5.5 Structure and bonding of boronitrides. (K1, K2, K3, K4, K5 & K6)

5.6 Metal clusters - chemistry of low molecularity metal clusters (up to trinuclear metal clusters). (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. J. E. Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper Collins, New York, 4th Edition, 2013.
2. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, John Wiley and Sons, 6th Edition, 2007.
3. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, WB Saunders Co., USA, 2010.
4. M. C. Day and J. Selbin, Theoretical Inorganic Chemistry, Van Nostrand Co., New York, 1974.
5. G. S. Manku, Inorganic Chemistry, Tata McGraw Hill Publications, 1989.
6. D. F. Shrivers, P. W. Atkins and C. H. Langford, Inorganic Chemistry, OUP, 2006.
7. N. H. Ray, Inorganic Polymers, Academic Press, 1978.
8. F. Basolo and R. G. Pearson, Mechanism of Inorganic Reaction, Wiley NY, 1967.

Open Educational Resources (OER):

1. https://nptel.ac.in/content/storage2/courses/104103071/pdf/mod2.pdf
2. https://nptel.ac.in/content/storage2/courses/104103069/module4/lec3/1.html
3. https://nptel.ac.in/courses/115/105/115105099/
4. http://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-11, M-19)

SEMESTER I

PCCHC20 - KINETICS AND PHOTOCHEMISTRY

Year: I SEM: I	Course Code PCCHC20	Title of the Course Kinetics and Photochemistry	Course Type Theory	Course Category Core	H/W 5	Credits 4	Marks 100

Learning Objectives:

- To get exposed to the kinetics of reactions in solutions, acid- base catalysis and surface reactions.
- To gain knowledge on photochemical and photo physical processes.
- To have an in-depth knowledge on the kinetics of complex and fast reactions.

Course Outcomes:

The Learners will be able to

1. Describe Activated Complex Theory in terms of translational and vibrational partition functions and apply it to derive the kinetics of reactions in solutions, Hammett and Taft equations and kinetic isotope effects in studying the mechanism of chemical reactions.
2. Discuss the concepts and kinetics of homogeneous and heterogeneous catalysis and explain adsorption isotherms of Langmuir and BET.
3. Derive the kinetics of complex reactions and apply the techniques of fast reactions.
4. Analyse the principles involved in photo excitation of molecules.
5. Derive the kinetics of photochemical reactions, and explain the applications of radiation chemistry, kinetics of photochemical reactions, solar energy conversion and radiolysis of water.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	M	H	H	H
CO2	H	H	M	H	H	H
CO3	H	H	M	H	H	H
CO4	H	H	M	H	H	H

CO5	H	H	M	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Activated complex theory - derivation - partition functions and activated complex - Eyring equation in terms of translational and vibrational partition functions. **(**KI, K2, K3, K4, K5 & K6)

1.2 Determination of free energy, enthalpy and entropy of activation and their significance. **(**KI, K2, K3, K4, K5 & K6)

1.3 Potential energy surfaces. **(**KI, K2, K3, K4, K5 & K6)

1.4 Applications of activated complex theory to reactions in solution - effect of pressure, and dielectric constant. **(**KI, K2, K3, K4, K5 & K6)

1.5 Effect of ionic strength on reactions in solutions, cage effect. **(**KI, K2, K3, K4, K5 & K6)

1.6 Kinetic isotope effect, linear free energy relationships - Hammett and Taft equations. **(**KI, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Catalysis - homogeneous catalysis - acid-base catalysis - types of acid-base catalysis - specific and general acid-base catalysis. Mechanisms and kinetics of acid-base catalyzed reactions (protolytic and prototropic mechanism) – Bronsted catalysis law. **((**KI, K2, K3, K4 & K5)

2.2 Heterogeneous catalysis - surface reactions, types - physisorption and chemisorption, difference between physisorption and chemisorption, Lennard-Jones plots. **(**KI, K2, K3, K4 & K5)

2.3 Adsorption isotherms - Langmuir and BET isotherms - postulates and derivations. **(**KI, K2, K3, K4 & K5)

2.4 Kinetics of surface reactions - unimolecular and bimolecular reactions, catalysis by semiconductor oxides (n-type and p-type). **(**KI, K2, K3, K4 & K5)

2.5 Mechanism of heterogeneous catalytic reactions, Langmuir and Rideal-Eley mechanism - adsorption co-efficient and its significance. **(**KI, K2, K3, K4 & K5)

2.6 Enzyme catalysis - types of enzyme catalysis, rate of enzyme catalyzed reactions by Michaelis-Menton mechanism - study of effect of substrate concentration, pH and temperature on enzyme catalyzed reactions - inhibition in enzyme catalyzed reactions. **(**KI, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Complex reactions - definition with examples, kinetics of reversible, consecutive and parallel reactions. **(**KI, K2, K3, K4, K5 & K6)

3.2 Chain reactions - types of chain reactions (stationary and non-stationary). **(**KI, K2, K3, K4, K5 & K6)

3.3 General treatment of chain reactions - chain length - explosion limits. **(**KI, K2, K3, K4, K5 & K6)

3.4 Rice Herzfeld mechanism - order of reactions of unity, one-half and three-halves for photolysis of acetaldehyde. **(**KI, K2, K3, K4, K5 & K6)

3.5 Fast reactions - relaxation methods - pressure and temperature jump methods **(**KI, K2, K3, K4, K5 & K6)

3.6 Stopped flow and flash photolysis methods. **(**KI, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Photochemistry - introduction, absorption and emission of radiation - intensity distribution in the electronic, vibrational species - Franck Condon Principle. **(**K1, K2, K3, K4 & K5)

4.2 Jablonski diagram - radiative and non-radiative processes - fluorescence and phosphorescence - E-type and P-type delayed fluorescence - spin forbidden radiative transition - internal conversion and intersystem crossing. **(**K1, K2, K3, K4 & K5)

4.3 Electronically excited states - excited state dipole moment and acidity constant. **(**KI, K2, K3, K4 & K5)

4.4 Decay of electronically excited states, dissociation and predissociation of diatomic molecules - energy transfer process. **(**KI, K2, K3, K4 & K5)

4.5 Photophysical processes - kinetics of unimolecular and bimolecular photophysical processes - kinetic treatment of excimer and exciplex formation. **(**KI, K2, K3, K4 & K5)

4.6 Quenching - static and dynamic quenching - Stern-Volmer equation. **(**KI, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Photochemical reactions - photo assisted mechanism, hydrogen and halogen reactions. **(**KI, K2, K3, K4, K5 & K6)

5.2 Kinetics of photochemical reaction, photoredox, photosubstitution, photoisomerization and photosensitized reactions. **(**KI, K2, K3, K4, K5 & K6)

5.3 Photovoltaic and photogalvanic cells, photo assisted electrolysis of water, application of solar energy conversion. **(**KI, K2, K3, K4, K5 & K6)

5.4 Radiation chemistry - interaction of high-energy radiation with matter - primary and secondary processes**. (**KI, K2, K3, K4, K5 & K6)

5.5 G value - radiolysis of water - hydrated electron, ion pair yield. **(**KI, K2, K3, K4, K5 & K6)

5.6 Photocatalysis - applications of TiO_2 photocatalyst for oxidation of organic pollutants - photochemical reaction of vision. **(**KI, K2, K3, K4, K5 & K6)

Reference Books:

1. R. G. Frost and Pearson, Kinetics and Mechanism, Wiley, New York, First Reprint 1970.
2. Keith J. Laidler, Chemical Kinetics, Pearson Edition Company Pvt. Ltd., 3rd Edition, 2005.
3. B. R. Puri, L. R. Sharma and M. S. Pathania, Principles of Physical Chemistry, Vishal Publishing Co., January 2019.
4. N. J. Turro, Modern Molecular Photo Chemistry, Benjamin, Cumming, Menlo Park, California, 1978.
5. K. K. Rohatgi Mukherjee, Fundamentals of Photo Chemistry, Wiley Eastern Ltd., 2nd Edition, 1992.
6. Gurdeep Raj, Photochemistry, Goel Publishing House, 4th Edition, 2002.
7. A. Singh, R. Singh, Photochemistry, Campus Books International, 1st Edition, 2005.
8. P. W. Atkins, Physical Chemistry, Oxford University Press, 11th Edition, 2018.

9. G. W. Castellan, Physical Chemistry, Narosa Publishing House, Seventh Reprint, 2004.
10. Donald A. Mc Quarrie and John D. Simon, Physical Chemistry: A Molecular Approach - 1997, Viva Books Pvt., Ltd., New Delhi, Reprint 2004.
11. J. Rajaram J.C. Kuriacose, Kinetics and Mechanisms of Chemical Transformations: Applications of Femto Chemistry, Mc Millan Publishers India Ltd., Reprint, 2009.

Open Educational Resources (OER):

1. http://photobiology.info/Ilichev.html (Photochemistry basics)
2. https://chem.libretexts.org/Courses/University_of_California_Davis/UCD_Chem_107B%3A_Physical_Chemistry_for_Life_Scientists/Chapters/2%3A_Chemical_Kinetics/2.10%3A_Fast_Reactions_in_Solution.
3. https://swayam.gov.in/nd1_noc20_cy22/preview (Introduction to Chemical Thermodynamics and Kinetics)
4. Brian Wardle, Principles and applications of photochemistry, Wiley publications, 2009, ISBN – 978-0-470-01494.

https://cds.cern.ch/record/1254287/files/9780470014936_TOC.pdf

SEMESTER I

PECHA20 - ELECTIVE I A: POLYMER CHEMISTRY

Year: I SEM: I	**Course Code** PECHA20	**Title of the Course** Polymer Chemistry	**Course Type** Theory	**Course Category** Core Elective	**H/W** 5	**Credits** 4	**Marks** 100

Learning Objectives:

- To gain knowledge on polymerization techniques and characterization of polymers.
- To get acquainted with the recent applications of polymers.

Course Outcomes:

The Learners will be able to

1. Classify polymers and illustrate the types of polymerization techniques.
2. Illustrate the characterization techniques such as XRD, TGA, DSC, SEM and TEM.
3. Discuss the polymer reactions and degradation.
4. Evaluate polymer processing techniques in industries, determine molecular weight of polymers by selected methods such as GPC, osmometry, viscometry, ultracentrifugation and MALDI methods.
5. Compile the synthesis, properties and applications of polymers and biopolymers.

CO	**PSO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	L	L	H	H	H
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CO3	H	M	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	L	M	H	H	H

CO	**PO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Introduction - basic concepts of polymer science - definitions, degree of polymerization, molecular forces, and chemical bonding in polymers. (K1, K2, K3, K4, K5 & K6)

1.2 Classification of polymers - natural and synthetic - organic and inorganic - thermoplastic and thermosetting polymers - plastics, elastomers, fibres and liquid resins. Linear, branched, and cross-linked polymers, addition polymers and condensation polymers. (K1, K2, K3, K4, K5 & K6)

1.1 Polymerization techniques - bulk, suspension, solution, and emulsion techniques. (K1, K2, K3, K4, K5 & K6)

1.2 Mechanism and kinetics of addition polymerization - cationic and anionic polymerization. (K1, K2, K3, K4, K5 & K6)

1.3 Mechanism and kinetics of free radical and condensation polymerization. (K1, K2, K3, K4, K5 & K6)

1.4 Co-ordination polymerization - mechanism using Ziegler Natta catalyst. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Characterization methods - crystalline nature - degree of crystallinity, degree of crystallisability and X-ray diffraction studies. (K1, K2, K3, K4 & K5)

2.2 Glass transition temperature (Tg) - definition, factors affecting glass transition temperature. (K1, K2, K3, K4 & K5)

2.3 Importance of glass transition temperature - relationship between glass transition temperature and melting point. (K1, K2, K3, K4 & K5)

2.4 Study of polymers - Differential Scanning Calorimetric (DSC) and Thermo Gravimetric Analysis of polymers (TGA). (K1, K2, K3, K4 & K5)

2.5 Relation to structure - surface morphology - Scanning Electron Microscopy (SEM). (K1, K2, K3, K4 & K5)

2.6 Size of the particle determination - Transmission Electron Microscopy (TEM). (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Polymer reactions - hydrolysis, acidolysis, hydrogenation, addition and substitution reactions. (K1, K2, K3, K4, K5 & K6)

3.2 Cyclisation, cross-linking and vulcanization. (K1, K2, K3, K4, K5 & K6)

3.3 Graft and block copolymers - definition and reactions leading to the formation of graft and block copolymers. (K1, K2, K3, K4, K5 & K6)

3.4 Types of degradation - chemical degradation, physical degradation, biodegradable polymers, and mechanism of degradation. (K1, K2, K3, K4, K5 & K6)

3.5 Thermal oxidation, photooxidation, mechanical degradation, degradation by ionizing radiation, ozone attack. (K1, K2, K3, K4, K5 & K6)

3.6 Degradation of special polymers: polyolefins, polyvinyl chloride (PVC) and polymethylmethaacrylate (PMMA). (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Physical properties, stress-strain behaviour, mechanical properties (tensile, flexural, impact, fatigue, hardness, creep, abrasion). (K1, K2, K3, K4 & K5)

4.2 Electrical properties (dielectric strength, surface resistivity, volume resistivity, power factor, arc resistance)**.** (K1, K2, K3, K4 & K5)

4.3 Polymer processing - films sheets: moulding - compression, blow moulding, injection moulding and extrusion moulding, casting of films and calendaring, recycling of plastics. (K1, K2, K3, K4 & K5)

4.4 Elastomers - introduction, processing, rubber types, vulcanization, properties, reclaiming. (K1, K2, K3, K4 & K5)

4.5 Fibers - introduction, production, fiber spinning, textile fibers, industrial fibers, recycling. (K1, K2, K3, K4 & K5)

4.6 Molecular weights of polymers - number average and weight average molecular weights, determination of molecular weight of polymers by viscometry, Gel Permeation Chromatography (GPC), membrane osmometry, vapour phase osmometry, ultracentrifugation, light scattering, and Matrix-Assisted Laser Desorption Ionization (MALDI) methods. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Applications of polymers - industrially important polymers - synthesis, properties and uses of natural and synthetic polymers. (K1, K2, K3, K4, K5 & K6)

5.2 Synthesis, properties and uses of polytetrafluoroethylene (Teflon), polystyrene, rayon, nylon, polyacrylates, polyvinyl chloride (PVA), polyacrylonitrile (PAN) and polystyrene-divinylbenzene. (K1, K2, K3, K4, K5 & K6)

5.3 Electrically conducting polymers - poly acetylene - poly aniline. (K1, K2, K3, K4, K5 & K6)

5.4 Biopolymers - natural - starch, cellulose, chitosan and silk and synthetic - polyvinyl alcohol (PVA), polyvinylpyrrolidone (PVP) and polylactic acid. (K1, K2, K3, K4, K5 & K6)

5.5 Biomedical application of biopolymers - dental materials, ophthalmology, orthopaedic implants, tissue engineering and drug delivery. (K1, K2, K3, K4, K5 & K6)

5.6 Industrial applications of biopolymers - packaging, automotive and electronics (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. V. R. Gowariker, N. V. Viswanathan and Jayadev Sridhar, Polymer Science, New Age International (P) Ltd., Reprint 2012.
2. F. W. Billmeyer, Textbook of Polymer Science, Wiley Inter Science, 3rd Edition, 2005.
3. Joel R., Polymer Science and Technology, Fried Prentice Hall, India, Reprint 2000.
4. G. S. Mishra, Introduction to Polymer Chemistry, Wiley Eastern Ltd., Reprint 2005.
5. M. G. Arora and M. Singh, Polymer Chemistry, Anmol Publications, Reprint 1996.
6. M. S. Bhatnagar, Textbook of Polymers, S. Chand and Company, First Edition, 2004.
7. R. J. Young and P. A. Lovell, Introduction to Polymers, Nelson Thornes Ltd., Reprint 2004.

Open Educational Resources (OER):

1. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P06 -Physical Chemistry-II-Macromolecules)
2. https://nptel.ac.in/courses/104/105/104105039/ (Polymer Chemistry)
3. https://chem.libretexts.org/Bookshelves/General_Chemistry/Book%3A_Chem1_(Lower)/07%3A_Solids_and_Liquids/7.09%3A_Polymers_and_Plastics
4. https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Supplemental_Modules_(Organic_Chemistry)/Polymers
5. https://ocw.mit.edu/courses/chemical-engineering/10-569-synthesis-of-polymers-fall-2006/lecture-notes/

SEMESTER I

PECHB20 - ELECTIVE I B: NANO CHEMISTRY

Year: I SEM: I	**Course Code** PECHB20	**Title of the Course** Nano Chemistry	**Course Type** Theory	**Course Category** Core Elective	**H/W** 5	**Credits** 4	**Marks** 100

Learning Objectives:

- To study the concepts in nano chemistry.
- To gain knowledge about characterization of nanoparticles by different techniques.
- To get exposed to the applications of nano chemistry.

Course Outcomes:

The Learners will be able to

1. Discuss the basic concepts of nano chemistry including theories of nano chemistry, and to classify the various types of nano systems.
2. Explain the different methods and techniques of synthesizing nanoparticles.
3. Discuss the characterization of the nanomaterials.
4. Explain the applications of nano chemistry in optics, electronics, and sensors.
5. Outline the biomedical application of nanoparticles.

CO	**PSO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	**PO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Fundamental science behind nano chemistry - scientific revolutions - nanosized effects - surface to volume ratio. (K1, K2, K3, K4, K5 & K6)

1.2 Atomic structure - molecules & phases - energy at the nanoscale, molecular and atomic size; quantum effects. (K1, K2, K3, K4, K5 & K6)

1.3 Classification based on the dimensionality - nanoparticles, nanoclusters, nanotubes, nanowires and nanodots. (K1, K2, K3, K4, K5 & K6)

1.4 Influence of nano structuring on mechanical, optical, electronic, magnetic and chemical properties. (K1, K2, K3, K4, K5 & K6)

1.5 Intermolecular forces, van der Waals' forces, dynamic properties of interfaces, contact angle, Brownian motion, and surface free energy. (K1, K2, K3, K4, K5 & K6)

1.6 Classical colloid theory - nucleation and growth, adsorption, and desorption kinetics - Ostwald ripening - homogeneous and heterogeneous nucleation. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Methods of synthesizing nanoparticles - top-down and bottom-up approach - grain growth - grain boundary - segregation, pinning and aggregation. (K1, K2, K3, K4 & K5)

2.2 Top-down methods - inert gas condensation, arc discharge, ion sputtering, laser pyrolysis, ball milling and Molecular Beam Epitaxy (MBE). (K1, K2, K3, K4 & K5)

2.3 Soft chemical methods - chemical precipitation and coprecipitation - metal nanocrystals - synthesis by polyol and borohydride reduction methods. (K1, K2, K3, K4 & K5)

2.4 Chemical vapour deposition (CVD) method, sol-gel synthesis, microemulsion synthesis, normal and reverse micelles formation, hydrothermal and solvothermal methods. (K1, K2, K3, K4 & K5)

2.5 Chemical processes - thermolysis routes, microwave assisted synthesis and Sono chemical assisted synthesis. (K1, K2, K3, K4 & K5)

2.6 Microbial routes - biosynthesis - template route, DC and pulsed electrodeposition and electroless deposition - combustion route. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 X-ray powder diffraction - quantitative determination of phases - structure analysis, particle size analysis using Scherer formula. (K1, K2, K3, K4, K5 & K6)

3.2 Thermal analysis methods - Thermo Gravimetric Analysis (TGA), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC). (K1, K2, K3, K4, K5 & K6)

3.3 Spectroscopy studies - Ultra Violet-Visible (UV), Fourier Transform Infrared spectroscopy (FTIR), Raman Spectroscopy and Photoluminescence Spectroscopy. (K1, K2, K3, K4, K5 & K6)

3.4 Microscopic techniques - optical microscope, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Atomic Force Microscopy (AFM). (K1, K2, K3, K4, K5 & K6)

3.5 Surface analysis and particle size - X-ray photoelectron spectroscopy, auger electron spectroscopy, zeta potential measurement and Dynamic Light Scattering (DLS) and ellipsometry. (K1, K2, K3, K4, K5 & K6)

3.6 Lithography - X-ray lithography, wet etching, dry etching, etch resists - dip pen lithography. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Zero-dimensional nanoparticles - quantum dots for solar cells, quantum dots for light emitting diode, molecular electronics, and nanoparticles as catalysts. (K1, K2, K3, K4 & K5)

4.2 Nanotube/nanowire-based field effect transistors for biosensing, gas sensing, piezoelectric nanowires as nanogenerator - carbon nanostructures - C60, C80, SWNT and MWNT. (K1, K2, K3, K4 & K5)

4.3 Nano porous anodized aluminum oxide, nano porous metal-organic framework for adsorption, separation and catalytic conversion of CO_2, nano porous materials for Li/Cd-ion battery applications. (K1, K2, K3, K4 & K5)

4.4 Nano sensors - optical, chemical, and physical sensors. (K1, K2, K3, K4 & K5)

4.5 Nano bioelectronics - DNA based biosensors, glucose sensors, protein-based biosensors and quantum dot based bioimaging. (K1, K2, K3, K4 & K5)

4.6 Nanoscale electronic devices - Complementary Metal Oxide Semiconductor (CMOS) and Magneto Resistive Random Access Memory (MRAM) devices. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Bio-medical applications - drug delivery - targeted drug delivery systems - various forms - liposomes, micelles, and dendrimers. (K1, K2, K3, K4, K5 & K6)

5.2 Photoablation therapy - photodynamic therapy and photo thermal therapy. (K1, K2, K3, K4, K5 & K6)

5.3 Cancer therapy - destruction of cancer cells with nanoparticles - magnetic hyperthermia. (K1, K2, K3, K4, K5 & K6)

5.4 Neuro electronic interface and nano luminescent tag. (K1, K2, K3, K4, K5 & K6)

5.5 Bioimaging, biosensors and biomass energy. (K1, K2, K3, K4, K5 & K6)

5.6 Genetic and tissue engineering. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. Cao, Guozhong, Nanostructures & Nanomaterials: Synthesis, Properties, and Applications, Imperial College Press, London, 2004.
2. Mickwilson, Basic Science and Emerging Technologies, Overseas Press, 2005.
3. Richard Booker and Earlboysen, Nano Technology, Willey Publication, 2005
4. Ratner, Nano Technology, Pearson Education, 2006.
5. K. Goser, Nano Electronics and Nano Systems, Springer International Edition, 2008.
6. W. R. Fahrner, Nano Technology and Electronics, Springer International Edition, 2008.
7. L. Daniel, Schodek, Paulo Ferreira, Michael F. Ash, Nanomaterials, Nanotechnologies and Design: An Introduction for Engineers, Elsevier, 2009.
8. G. A. Ozin, A. C. Arsenault, and L. Cademartiri, Nanochemistry: A Chemical Approach to Nanomaterials, The Royal Society of Chemistry, Cambridge, 2nd Edition, 2009.

Open Educational Resources (OER):

1. https://nptel.ac.in/courses/118/104/118104008/(Nanostructures and Nanomaterials)
2. https://nptel.ac.in/courses/118/102/118102003/ (Nanotechnology)
3. https://chem.libretexts.org/Bookshelves/General_Chemistry/Map%3A_Chemistry__The_Central_Science_(Brown_et_al.)/12%3A_Solids_and_Modern_Materials/12.6%3A_Materials_for_Nanotechnology
4. https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Book%3A_Introduction_to_Inorganic_Chemistry/11%3A_Basic_Science_of_Nanomaterials
5. https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-701-introduction-to-nanoelectronics-spring-2010/

SEMESTER II

PCCHD20 - ORGANIC REACTIONS AND MECHANISMS

Year: I SEM: II	Course Code PCCHD20	Title of the Course Organic Reactions and Mechanisms	Course Type Theory	Course Category Core	H/W 4	Credits 4	Marks 100

Learning Objectives:

- To discuss the various oxidation and reduction reactions.
- To understand the mechanisms of rearrangements.
- To learn about photochemical and pericyclic reactions.

Course Outcomes:

The Learners will be able to

1. Discuss the oxidation of organic compounds using selected oxidizing reagents.
2. Discuss the reduction of organic compounds using selected reducing reagents.
3. Describe the mechanisms of various rearrangement reactions and their applications.
4. Explain the reaction mechanisms and applications of selected named reactions.
5. Illustrate the types of photo chemical reactions, classify pericyclic reactions, and examine the correlation diagram for butadiene-cyclobutene system.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(12 Hours)**

1.1 Oxidation by quinones and selenium dioxide. (K1, K2, K3, K4, K5 & K6)
1.2 Oxidation by osmium tetroxide and lead tetraacetate. (K1, K2, K3, K4, K5 & K6)
1.3 Formation of C-C bond in phenol coupling and acetylenic coupling. (K1, K2, K3, K4, K5 & K6)
1.4 Oxidation by chromic acid (Jones reagent) and chromium trioxide - pyridine (Sarett's reagent), ozone, hydrogen peroxide and potassium permanganate. (K1, K2, K3, K4, K5 & K6)
1.5 DMSO-DCC (Pfitzer-Moffatt reagent) and Oppenauer oxidation. (K1, K2, K3, K4, K5 & K6)
1.6 Dakin reaction and Swern oxidation. (K1, K2, K3, K4, K5 & K6)

Unit II **(12 Hours)**

2.1 Catalytic reduction - hydrogenation, hydrogenolysis - reduction by metals (Cu, Pd, Ni). (K1, K2, K3, K4 & K5)
2.2 Wolf- Kishner reduction and its modification and Clemmensen reduction. (K1, K2, K3, K4 & K5)
2.3 Birch and MPV reduction reactions. (K1, K2, K3, K4 & K5)
2.4 Reduction of carbonyl compounds (aldehydes and ketones) with $LiAlH_4$ and $NaBH_4$. (K1, K2, K3, K4 & K5)
2.5 Reduction of carbonyl compounds (aldehydes and ketones) with tritertiary butoxyaluminium hydride and sodium cyanoborohydride. (K1, K2, K3, K4 & K5)
2.6 Selectivity in reduction of 4-t-butylcyclohexanone using selected hydrides. ($LiAlH_4$ and $NaBH_4$) (K1, K2, K3, K4 & K5)

Unit III **(12 Hours)**

3.1 A detailed study with suitable examples of the mechanism of the following rearrangements - Wagner-Meerwein and Demjanov rearrangements. (K1, K2, K3, K4, K5 & K6)
3.2 Dienone - Phenol and Favorski rearrangements. (K1, K2, K3, K4, K5 & K6)
3.3 Baeyer-Villiger and Wolf rearrangements. (K1, K2, K3, K4, K5 & K6)
3.4 Von-Richter and Curtius rearrangements. (K1, K2, K3, K4, K5 & K6)
3.5 Lossen and Schmidt rearrangements. (K1, K2, K3, K4, K5 & K6)
3.6 Nitrenes - singlet and triplet nitrenes. Methods of generating nitrenes and their reactions. (K1, K2, K3, K4, K5 & K6)

Unit IV **(12 Hours)**

4.1 Reaction mechanism and applications of Barton and Simmons-Smith reactions. (K1, K2, K3, K4 & K5)
4.2 Reaction mechanisms and applications of Stobbe condensation and Mannich. (K1, K2, K3, K4 & K5)
4.3 Darzen condensation and Chichibabin reactions. (K1, K2, K3, K4 & K5)
4.4 Reaction mechanisms and applications of Michael addition and Skraup synthesis. (K1, K2, K3, K4 & K5)
4.5 Reaction mechanisms and applications of Hunsdiecker and Ullmann reactions. (K1, K2, K3, K4 & K5)

4.6 Reaction mechanisms and applications of Nef and HVZ. (K1, K2, K3, K4 & K5)

Unit V **(12 Hours)**

5.1 Photochemical excitation - fate of the excited molecules - Jablonski diagram - study of photo chemical reaction of ketone. (K1, K2, K3, K4, K5 & K6)

5.2 Norrish type I and Norrish type II reactions. (K1, K2, K3, K4, K5 & K6)

5.3 Photocycloaddition - Paterno-Buchi reduction - photo cycloaddition of α-β unsaturated ketones- di-pi methane rearrangement. (K1, K2, K3, K4, K5 & K6)

5.4 Pericyclic reactions - classification, orbital symmetry - Woodward Hoffmann rules. (K1, K2, K3, K4, K5 & K6)

5.5 Analysis of electrocyclic reactions - types - 4n and 4n + 2 systems - cyclo addition – types – [2+2] and [4+2] cycloaddition reactions. Sigmatropic reactions - 1, n hydrogen shift, Cope rearrangement and Claisen rearrangement. (K1, K2, K3, K4, K5 & K6)

5.6 Correlation diagrams for butadiene - cyclobutene system. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. R. O. C. Norman & Coxon, Principles of Organic Chemistry, New York, 3rd Edition, Reprint 2012.
2. Francis A. Carey and Richard J, Sundberg, Part B-Advanced Organic Chemistry Kluwer Academic Publishers, 5th Edition, Reprint 2007.
3. S. M. Mukherji and S. P. Singh, Organic Reaction Mechanism, Mac Millan India Ltd., Chennai, 3rd Edition, Reprint 2010.
4. Sanyal S. N. Bharathi Bhawan, Reactions, Rearrangements and Reagents, Reprint 2019.
5. Jerry March, Advanced Organic Chemistry, Wiley Inter Science, 4th Edition, Reprint 2015.
6. P. S. Kalsi, Stereochemistry and Mechanism Through Solved Problems, Wiley Eastern Ltd., Reprint 2018.
7. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 4th Edition, Reprint 2015.
8. P. S. Kalsi, Organic Reaction and their Mechanism, New Age International Limited, Reprint 2017.
9. V. K. Ahluwalia, Organic Reaction Mechanisms, Narosa Publishing House, 2nd Edition, 2018.
10. R. K. Mackie and D. M. Smith, Organic Synthesis, Longman Publication, Reprint 1983.
11. P. S. Kalsi, Stereochemistry Conformation and Mechanism, New Age International (P) Ltd., Reprint 2017.
12. Jagdamba Singh and Jaya Singh, Photochemistry and Pericyclic Reactions, New Age International Publishers, 3rd Edition, 2019.
13. Dr. Raj K. Bansal, Organic Reaction Mechanisms, Tata Mc Graw- Hill Publishing Company Ltd., 4th Reprint 2012.

OER:

1. https://nptel.ac.in/courses/104/105/104105038/
2. https://nptel.ac.in/content/storage2/courses/104103022/download/module8.pdf
3. https://nptel.ac.in/courses/104/103/104103023/
4. https://nptel.ac.in/courses/104/103/104103023/

SEMESTER II

PCCHE20 - ADVANCED COORDINATION CHEMISTRY

Year: I SEM: II	Course Code PCCHE20	Title of the Course Advanced Coordination Chemistry	Course Type Theory	Course Category Core	H/W 5	Credits 4	Marks 100

Learning Objectives:

- To have an in-depth knowledge on coordination chemistry, stability of the complexes and stereochemistry of complexes.
- To study about the crystal field theory and applications of inorganic complexes.
- To gain knowledge about the concepts of electron transfer and substitution reactions.

Course Outcomes:

The Learners will be able to

1. Interpret the stability of complexes and explain the applications of various macrocyclic ligands.
2. Explain and analyse the concepts of CFT, MOT and Jahn Teller distortion.
3. Analyse the absorption spectra and determine magnetic susceptibility of metal complexes by different methods.
4. Discuss the electron transfer reaction mechanisms and their importance in biological systems.
5. Explain the reactivity and mechanisms of square planar and octahedral complexes and appraise the applications of complexes in various fields.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	M	M	H
CO2	H	M	H	M	M	H
CO3	H	H	H	H	M	H
CO4	H	M	L	M	H	H
CO5	H	M	M	M	M	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	M	L	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	M	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Thermodynamic and kinetic stability - stepwise and overall stability constants - relationship between both the constants. (K1, K2, K3, K4, K5 & K6)

1.2 Trend in K-value - Irving-Williams series - classification of metals. (K1, K2, K3, K4, K5 & K6)

1.3 Factors affecting the stability of complexes. (K1, K2, K3, K4, K5 & K6)

1.4 Determination of stability constants by spectrophotometric, polarographic and potentiometric methods - detection of complex formation. (K1, K2, K3, K4, K5 & K6)

1.5 Optical rotatory dispersion and circular dichroism - application to complexes. (K1, K2, K3, K4, K5 & K6)

1.6 Macrocyclic ligands: thermodynamic and kinetic template effect - structure, stability and applications of porphyrins, corrins, Schiff bases, crown ethers and crypts. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 CFT - salient features of CFT, crystal field splitting of d-orbitals in octahedral complexes - factors affecting the magnitude of Δ_o, crystal field splitting of d-orbitals in tetrahedral, tetragonal, and square planar complexes. (K1, K2, K3, K4 & K5)

2.2 Consequences of CF splitting - formation of high-spin and low-spin complexes, distribution of d-electrons. (K1, K2, K3, K4 & K5)

2.3 CFSE - calculation of CFSE for various d systems in O_h and T_d fields - uses of CFSE values, applications of CFT, limitations. (K1, K2, K3, K4 & K5)

2.4 Jahn-Teller distortion - theorem, z-in and z-out cases, causes and consequences. (K1, K2, K3, K4 & K5)

2.5 MOT - experimental evidences for metal-ligand covalent bonding in complexes, σ–bonding in O_h complexes - construction of MO diagrams. (K1, K2, K3, K4 & K5)

2.6 Pi-bonding in O_h complexes, effect of π–bonding on the value of Δ_o, relation between pi bonding ability of ligands and spectrochemical series, comparison of CFT with MOT. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Types of absorption spectra - ligand spectra, counter - ion spectra, CT spectra, ligand field spectra - R-S coupling. (K1, K2, K3, K4, K5 & K6)

3.2 Microstates - spectroscopic terms - ground state term: Hund's rule - term states for 'd' - ions. (K1, K2, K3, K4, K5 & K6)

3.3 Selection rules - Laporte's and spin selection rules, splitting of terms in octahedral and tetrahedral complexes. (K1, K2, K3, K4, K5 & K6)

3.4 Correlation diagrams - Orgel diagrams and Tanabe-Sugano diagrams - important features - spectra of different d systems - Racah parameters - nephelauxetic effect. (K1, K2, K3, K4, K5 & K6)

3.5 Charge transfer spectra - classification - ligand to metal, metal to ligand, inter valence and intra ligand charge transfer. (K1, K2, K3, K4, K5 & K6)

3.6 Magnetic characteristics of transition metal complexes - types of magnetic character - determination of magnetic susceptibility - Gouy and Faraday's method -magnetic properties of complex ions - magnetic criterion of bond type in complex and orbital contribution to magnetic moment. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Electron transfer reactions (redox reactions): Outer Sphere Mechanism - characteristics, factors influencing OSM. (K1, K2, K3, K4 & K5)

4.2 Cross reactions - Marcus-Hush principle. Inner Sphere Mechanism - characteristics. (K1, K2, K3, K4 & K5)

4.3 Inner Sphere Mechanism - factors influencing ISM, OSM versus ISM. (K1, K2, K3, K4 & K5)

4.4 Two electron transfers, non-complementary electron transfer reactions, reactions of the coordinated ligands, geometrical and optical isomerization reactions. (K1, K2, K3, K4 & K5)

4.5 Electron transfer reactions in biological systems - cytochromes, rubredoxins and ferredoxins. (K1, K2, K3, K4 & K5)

4.6 Ligand substitution reactions in square-planar complexes - mechanism - influences of entering, leaving and central metal ion on the reactivity of square planar complexes of Pt (II). (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Trans effect - trans effect series - theories and applications, cis effect. (K1, K2, K3, K4, K5 & K6)

5.2 Mechanisms of substitutions in octahedral complexes - dissociative, associative and interchange (I_a and I_d) mechanisms. (K1, K2, K3, K4, K5 & K6)

5.3 Hydrolysis reactions - acid hydrolysis and base hydrolysis reactions of six-coordinated Co(III) ammine complexes - mechanisms - evidences. (K1, K2, K3, K4, K5 & K6)

5.4 Replacement of coordinated water - mechanisms - evidences - rates of water replacement - orbital occupation effects. (K1, K2, K3, K4, K5 & K6)

5.5 Synthesis of coordination compounds by substitution reactions - chemistry of Pt and Co compounds. (K1, K2, K3, K4, K5 & K6)

5.6 Metal complexes in medicinal chemistry, industrial processes, and agriculture. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, WB Saunders Co., USA, Indian Edition, Reprint 2012.
2. J. E. Huheey, Inorganic Chemistry, Harper and Collins, NY, 4th Edition, Reprint 2006.
3. F. A. Cotton and G. W. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, John Wiley and Sons, 6th Edition, Reprint 2007.
4. R. Gopalan, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., Reprint 2008.
5. B. E. Douglas DH McDaniel's and Alexander, Concepts and Models of Inorganic Chemistry, Wiley Publication, 3rd Edition, Reprint 2006.
6. Wahid U. Malik, G. D. Tuli, R. D. Madan, Selected Topics in Inorganic Chemistry, S. Chand and Co., New Delhi, Reprint 2010.
7. S. F. A. Kettle, Coordination Chemistry, ELBS, Reprint 1990.
8. M. C. Shrivers, P. W Atkins, C. H. Langford, Inorganic Chemistry, Oxford University Press, 6th Edition, Reprint 2014.

9. G. S. Manku, Theoretical Principles of Inorganic Chemistry, Tata McGraw-Hill Publishers, Reprint 2011.

OER:

1. http://wwwchem.uwimona.edu.jm/courses/IC10Kout.html
2. https://ocw.mit.edu/courses/chemistry/5-04-principles-of-inorganic-chemistry-ii-fall-2008/
3. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-03, P-07)
4. https://nptel.ac.in/courses/104/101/104101116/ (Electron Transfer (ET) in living systems)

SEMESTER II

PCCHF20 - GROUP THEORY AND QUANTUM CHEMISTRY

Year: I SEM: II	Course Code PCCHF20	Title of the Course Group Theory and Quantum Chemistry	Course Type Theory	Course Category Core	H/W 5	Credits 4	Marks 100

Learning Objectives:

- To learn the concepts of Group theory and its applications.
- To study the fundamental principles of Quantum Chemistry, Schrodinger wave equation and its applications.
- To understand the application of Quantum Chemistry to chemical bonding.

Course Outcomes:

The Learners will be able to

1. Identify symmetry operations and assign point groups of molecules.
2. Construct the character tables for C_{2v} and C_{3v} point groups, apply the concepts of symmetry in molecular vibrations, chemical bonding, and electronic transitions.
3. Identify the limitations of classical mechanics, apply quantum chemistry to solve Schrödinger wave equation for one, two- and three-dimensional boxes and for hydrogen atom and helium ion.
4. Discuss classical and quantum mechanical treatments of one-dimensional harmonic oscillator, calculate the rotational constant and bond length of diatomic molecules.
5. Discuss and apply the approximation methods to single and multi-electron systems, apply the MO theory to di and polyatomic molecules, explain the application of HMO theory to ethylene, butadiene, and benzene.

CO	PSO					
	1	2	3	4	5	6
CO1	H	M	H	M	H	M
CO2	H	M	M	M	H	L
CO3	H	M	M	M	H	L
CO4	H	M	M	M	H	L
CO5	H	M	M	M	H	L

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	M	H
CO2	H	H	H	H	L	H
CO3	H	H	H	H	L	H
CO4	H	H	H	H	L	H
CO5	H	H	H	H	L	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Introduction - symmetry elements and symmetry operations, group postulates and types of groups, sub groups, abelian and non-abelian groups. (K1, K2, K3, K4, K5 & K6)

1.2 Group multiplication table, similarity transformations and classes of symmetry operations. (K1, K2, K3, K4, K5 & K6)

1.3 Molecular point groups - point groups of molecules, point groups of tetrahedral and octahedral molecules. Identification of symmetry operations and determination of point groups. (K1, K2, K3, K4, K5 & K6)

1.4 Matrices - matrix representations of symmetry operations, reducible and irreducible representations. (K1, K2, K3, K4, K5 & K6)

1.5 Orthogonality theorem and its consequences, properties of irreducible representations, labeling of irreducible representations. (K1, K2, K3, K4, K5 & K6)

1.6 Crystallographic symmetry - the 32 crystallographic point groups - space groups - screw axis - glide planes - comparison of crystallographic symmetry with molecular symmetry. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Construction of character table for C_{2V} and C_{3V} point groups - explanation for the complete character table for C_{2V} and C_{3V} point groups. (K1, K2, K3, K4 & K5)

2.2 Selection rules for vibrational IR and Raman spectra. (K1, K2, K3, K4 & K5)

2.3 Mutual exclusion rule for molecules with centre of symmetry. (K1, K2, K3, K4 & K5)

2.4 Applications to molecular vibrations (IR and Raman) for determining symmetry of normal modes of vibration in nonlinear molecules H_2O, CH_4, BF_3 and NH_3 using group theory. (K1, K2, K3, K4 & K5)

2.5 Hybrid orbitals in nonlinear molecules CH_4, XeF_4, BF_3, SF_6, NH_3. (K1, K2, K3, K4 & K5)

2.6 Application of group theory to electronic spectra of ethylene and formaldehyde. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Introduction to quantum mechanics - black body radiation - distribution of energy in the black body radiation - Rayleigh Jeans' and Planck's law of radiation. (K1, K2, K3, K4, K5 & K6)

3.2 Photoelectric effect, Bohr's quantum theory and subsequent developments - duality of electron and Compton Effect. (K1, K2, K3, K4, K5 & K6)

3.3 Quantum theory - quantum mechanical postulates – operators - definition, types of operators and Hermitian property. (K1, K2, K3, K4, K5 & K6)

3.4 Particle in a box model (one-, two- and three-dimensional cases). (K1, K2, K3, K4, K5 & K6)

3.5 Schrodinger equation for hydrogen atom and He^+ ion. (K1, K2, K3, K4, K5 & K6)

3.6 Origin of quantum numbers and their significance. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 One dimensional harmonic oscillator - classical treatment and quantum mechanical treatment. (K1, K2, K3, K4 & K5)

4.2 Normalization and the characteristics of the Eigen functions of a harmonic oscillator. (K1, K2, K3, K4 & K5)

4.3 The recursion formula for the Hermite polynomials, selection rules of the harmonic oscillator and space quantization of electronic orbitals. (K1, K2, K3, K4 & K5)

4.4 Rotation of diatomic molecules - wave equation and solution of the rigid rotor. (K1, K2, K3, K4 & K5)

4.5 Schrodinger wave equation and solution of particle in a ring. (K1, K2, K3, K4 & K5)

4.6 Calculation of rotational constants and bond lengths of diatomic molecules. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Approximation methods - variation methods - trial wave function - application of variation method to hydrogen and helium atoms. (K1, K2, K3, K4, K5 & K6)

5.2 Perturbation method and its application to particle in one dimensional box. (K1, K2, K3, K4, K5 & K6)

5.3 Born Oppenheimer approximation - treatment of molecules - application to helium atom. (K1, K2, K3, K4, K5 & K6)

5.4 Hydrogen molecule - Heiter-London theory or valence bond treatment - energy level diagram. (K1, K2, K3, K4, K5 & K6)

5.5 Linear Combination of Atomic Orbitals (LCAO) - molecular orbital theory for hydrogen molecule ion and hydrogen molecule. (K1, K2, K3, K4, K5 & K6)

5.6 Huckel's theory for conjugated molecules - ethylene, butadiene and benzene - semi empirical methods - Slater orbital and Hartree Fock–Self Consistent Field (HFSCF) methods. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. R. K. Prasad, Quantum Chemistry, New Age International (P) Ltd. Publishers, New Delhi, 3rd Edition, 2006.
2. D. A. Mcquarrie, Quantum Chemistry, University Science Books, Mill Valley, California, Reprint 2007.
3. R. Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India Ltd., 2001.
4. Ira N. Levine, Quantum Chemistry, Prentice Hall of India, New Delhi, 5th Edition, 2006.
5. Mahendra R. Awode, Quantum Chemistry, S. Chand & Company Ltd., New Delhi, 2002.
6. A. K. Chandra, Quantum Chemistry, Tata McGraw-Hill Publishing Company, New Delhi, 10th Edition, 2008.
7. Melvin W. Hanna, Quantum Mechanics in Chemistry, The Benjamin / Cummings Publishing Company, 2nd Edition, 1969.
8. K. V. Raman, Group Theory and Its Applications to Chemistry, Tata McGraw-Hill Publishing Company Ltd., Reprint 2004.
9. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishing Co., Reprint 2005.
10. F. A. Cotton, Group Theory and Its Applications to Chemistry, John Wiley & Sons (Asia) Pvt. Ltd., Singapore, 2004.
11. A. Salahuddin Kunju and G. Krishnan, Group theory and its Applications in Chemistry, Asoke K. Ghosh, PHI Learning Pvt. Ltd., New Delhi, 2010.

OER:

1. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-02 PhysicalChemistry-1 Quantum Chemistry)
2. https://symotter.org/ (Group Theory)
3. https://nptel.ac.in/courses/104/106/104106074/ (Quantum Chemistry)
4. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-13 Applications of molecular symmetry and Group Theory)
5. https://nptel.ac.in/courses/104/104/104104080/ (Chemical applications of group theory)

SEMESTER II

PECHC20 - ELECTIVE II A: PHARMACEUTICAL CHEMISTRY

Year: I SEM: II	Course Code PECHC20	Title of the Course Pharmaceutical Chemistry	Course Type Theory	Course Category Core Elective	H/W 5	Credits 4	Marks 100

Learning Objectives:

- To learn about the drugs, metabolism and the side effects.
- To understand the importance of drug design and development of drugs.
- To know the cancer and the drugs used.
- To learn about the various nutraceuticals and anticoagulants.

Course Outcomes:

The Learners will be able to

1. Classify the pharmaceutical drugs and explain the mechanism of drug action and absorption of drugs.
2. Elaborate the biological role of important inorganic compounds and the drugs used in the treatment of mental disorders.
3. Summarize the methods of drug design and development.
4. Review the causes of cancer and its treatment, and to assess the mechanism and the mode of action of anticancer drugs.
5. Formulate the different types of Nutraceuticals and their applications, and to justify the role of anticoagulants in the treatment of blood disorder.

CO	PSO					
	1	2	3	4	5	6
CO1	H	M	L	H	H	H
CO2	H	M	L	H	H	H
CO3	H	M	L	H	H	H
CO4	H	M	L	H	H	H
CO5	H	M	L	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Classification of drugs: biological, chemical, commercial consideration and lay public. (K1, K2, K3, K4, K5 & K6)

1.2 Mechanism of drug action and metabolism of drugs - mechanism of action, drug receptors binding, biological responses - covalent bond, hydrogen bond, van der Waal's forces. (K1, K2, K3, K4, K5 & K6)

1.3 Metabolism of drugs - chemical pathways - phase I and phase II reactions, biotransformation. (K1, K2, K3, K4, K5 & K6)

1.4 Routes of administration of drugs. (K1, K2, K3, K4, K5 & K6)

1.5 Absorption of drugs - factors affecting absorption. (K1, K2, K3, K4, K5 & K6)

1.6 Digestion and absorption of proteins and fats. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Assay of drugs - chemical, biological, and immunological assay. (K1, K2, K3, K4 & K5)

2.2 Psychopharmacology - antipsychotic drugs, phenothiazines, LSD, marijuana. (K1, K2, K3, K4 & K5)

2.3 Barbiturates - mechanism of action. (K1, K2, K3, K4 & K5)

2.4 Biological role of some inorganic compounds - sodium and potassium and their compounds. (K1, K2, K3, K4 & K5)

2.5 Calcium and iodine and their compounds. (K1, K2, K3, K4 & K5)

2.6 Copper and zinc and their compounds. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Drug design and development - introduction, discovery of drugs and lead compounds, different approaches to find lead compounds. (K1, K2, K3, K4, K5 & K6)

3.2 Development of drugs: Lead modification - pharmacophore modification, modification of structure or functional group, Structure Activity Relationship (SAR) - Prontosil, Streptomycin. (K1, K2, K3, K4, K5 & K6)

3.3 Structure modification methodologies to increase potency - homologation, chain branching, ring-chain transformation, extension of structure, isosteres and bioisosteres. (K1, K2, K3, K4, K5 & K6)

3.4 Quantitative Structure Activity Relationship (QSAR) - Hammett equation (electronic effects), Taft Equation (steric effects), Hansch equation (lipophilicity effect), Hansch analysis. (K1, K2, K3, K4, K5 & K6)

3.5 Craig plot, drug design using QSAR. (K1, K2, K3, K4, K5 & K6)

3.6 Computer assisted drug design (CADD). (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Cancer chemotherapy - terms used - types of neoplasms, stages of cancer, metastasis, and difference between cancer and normal cells. (K1, K2, K3, K4 & K5)

4.2 Tumor formation mechanism, causes of cancer, ways of reducing the risks. (K1, K2, K3, K4 & K5)

4.3 Treatment of cancer - radiation, surgery, chemotherapy, photodynamic therapy (PDT), immunotherapy, combined therapy, actions of antitumor agents. (K1, K2, K3, K4 & K5)

4.4 Determination of drug response - growth fraction, the mass doubling time, total tumor burden, tumor heterogeneity, cell cycle phase**,** drug resistance, host factors. (K1, K2, K3, K4 & K5)

4.5 Cytotoxic anticancer drugs - alkylating agents (Mustards) and their modes of action, antimetabolites - folic acid antagonist, purine antagonist and their modes of action. (K1, K2, K3, K4 & K5)

4.6 Pyrimidine agents and their modes of action, antitumor antibiotics and their modes of action, plant products, podophyllotoxins and their modes of action, endocrine agents and their modes of action, miscellaneous anticancer agents. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Nutraceuticals - introduction, types - plant sources. (K1, K2, K3, K4, K5 & K6)

5.2 Animal sources, microbial sources, nutraceuticals derived from all sources. (K1, K2, K3, K4, K5 & K6)

5.3 Antioxidants - definition, examples, role of antioxidants. (K1, K2, K3, K4, K5 & K6)

5.4 Toxins and their medicinal values - introduction, classification of toxins, toxins from reptiles and animals. (K1, K2, K3, K4, K5 & K6)

5.5 Toxins from insects, plants, marine origin, and microorganisms. (K1, K2, K3, K4, K5 & K6)

5.6 Anticoagulants - blood coagulation pathway, prevention of coagulation, direct and indirect acting anticoagulants, and anticoagulation therapy. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. V. K. Ahluwalia, Madhu Chopra, Medicinal Chemistry, ANE Books India, 2008.
2. Jayashree Ghosh, Fundamental Concepts of Applied Chemistry, S. Chand Company Ltd., 2nd Edition, 2006.
3. Graham L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, 6th Edition, Reprinted 2017.
4. David A. Williams, Foye's Principles of Medicinal Chemistry, Lippincott Williams and Wilkins, 2012.
5. Asuthosh Kar, Medicinal Chemistry, New Age International Publishers, New Delhi, 7th Edition, 2018.
6. N. K. Jain, Progress in Controlled and Novel Drug Delivery Systems, CBS Publishers & Distributors, New Delhi, 2013.
7. P. S. Kalsi and Sangeeta Jagtap, Pharmaceutical, Medicinal and Natural Product Chemistry, Narosa Publishing House, New Delhi, 2013.

OER:

1. https://opentextbc.ca/anatomyandphysiology/chapter/18-5-hemostasis/
2. https://nptel.ac.in/courses/102/106/102106070/

SEMESTER II

PECHD20 - ELECTIVE II B: MEDICINAL CHEMISTRY

Year: I SEM: II	Course Code PECHD20	Title of the Course Medicinal Chemistry	Course Type Theory	Course Category Core Elective	H/W 5	Credits 4	Marks 100

Learning Objectives:

- To have a clear understanding about drug designing and the principles involved in it.
- To deepen the knowledge on biochemical considerations of drug designing.

Course Outcomes:

The Learners will be able to

1. Explain the designing of drugs by different approaches.
2. Define the physiochemical properties of drug molecules, and illustrate pharmacophore, toxicophore, metabophore and interchangeable bioisosteres.
3. Describe the nature of drug receptors and their binding interactions.
4. Explain the stereochemical properties and biological activity of drug molecules, and to identify the properties of drug molecules by quantum mechanics and molecular mechanics.
5. Describe the physiological and pathological approaches while designing newer drugs for newer diseases, and to Discuss the biological activity of steroids and radioisotopes.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Drug design - rational approach and conceptual approach. (K1, K2, K3, K4, K5 & K6)

1.2 Practical approach and humanitarian approach. (K1, K2, K3, K4, K5 & K6)

1.3 The method of variation. (K1, K2, K3, K4, K5 & K6)

1.4 Drug design through disjunction and conjunction. (K1, K2, K3, K4, K5 & K6)

1.5 Research and development strategies. (K1, K2, K3, K4, K5 & K6)

1.6 Molecular hybridization, rigidity, and flexibility versus drug design, tailoring of drugs. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Definition and properties of drug molecules. (K1, K2, K3, K4 & K5)

2.2 Physiochemical properties of drug design. (K1, K2, K3, K4 & K5)

2.3 Structural integrity of drug molecules. (K1, K2, K3, K4 & K5)

2.4 Pharmaceutical, pharmacokinetics and pharmacodynamic phases. (K1, K2, K3, K4 & K5)

2.5 Structural fragments of drug molecules - pharmacophore and toxicophore. (K1, K2, K3, K4 & K5)

2.6 Metabophores and interchangeable bioisosteres. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 The receptor concept - the nature of receptors and criteria for receptor identity. (K1, K2, K3, K4, K5 & K6)

3.2 Definitions of drug - receptor binding interactions. (K1, K2, K3, K4, K5 & K6)

3.3 Selection of drug - receptor binding forces in drug design. (K1, K2, K3, K4, K5 & K6)

3.4 General molecular concepts of drug receptor action, functional molecular properties of drug receptors. (K1, K2, K3, K4, K5 & K6)

3.5 Definition of classical binding terms for drug - receptor interactions. (K1, K2, K3, K4, K5 & K6)

3.6 The clinical-molecular interface: The concept of rational poly pharmacy - drug-drug interactions in drug design. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Structure and properties of drug molecules. (K1, K2, K3, K4 & K5)

4.2 Conformational, topological, and steric properties of drug molecules. (K1, K2, K3, K4 & K5)

4.3 Enantiomers and diastereomers of drug molecules. (K1, K2, K3, K4 & K5)

4.4 Stereochemistry and biological activity of drug molecules. (K1, K2, K3, K4 & K5)

4.5 Electronic properties of drug molecules. (K1, K2, K3, K4 & K5)

4.6 Predicting the properties of drug molecules - quantum mechanics and molecular mechanics. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Biochemical considerations in drug design - the physiological and pathological approaches. (K1, K2, K3, K4, K5 & K6)

5.2 Newer drugs for newer diseases - introduction, newer drugs. (K1, K2, K3, K4, K5 & K6)

5.3 Hormone antagonists - anti estrogen - aldosterone antagonists. (K1, K2, K3, K4, K5 & K6)

5.4 Anti progestational steroids - cardiac steroids and related inotropic drugs. (K1, K2, K3, K4, K5 & K6)

5.5 Cardiac steroids, phosphodiesterase inhibitors, adenylate cyclase stimulants, drugs that enhance the Ca^{2+} sensitivity of myocardial contractile proteins. (K1, K2, K3, K4, K5 & K6)

5.6 Radio sensitizer - therapeutic radioisotopes, imaging radioisotopes - drugs to combat AIDS. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. Thomas Nogrady, Dona Id F. Weaver, Medicinal Chemistry: A Molecular and Biochemical Approach, Oxford University Press, Third Edition, 2005.
2. V. K. Ahluwalia, Madhu Chopra, Medicinal Chemistry, Ane Books India, 2008.
3. D. Sriram, P. Yogeeswari, Medicinal Chemistry, Pearson Education, 2007.
4. Asuthosh Kar, Medicinal Chemistry, New Age International Publishers, New Delhi, 7^{th} Edition, 2018.

OER:

1. http://epj.eg.net/article.asp?issn=1687-4315;year=2013;volume=12;issue=2;spage=95;epage=108;aulast=Kamel;type=3
2. https://www.britannica.com/science/steroid/Steroid-numbering-system-and-nomenclature
3. https://nptel.ac.in/courses/102/106/102106070/

SEMESTER II

PCCHG20 - PRACTICAL I: ORGANIC CHEMISTRY - I

Year: I SEM: II	Course Code PCCHG20	Title of the Course Practical I: Organic Chemistry – I	Course Type Practical	Course Category Core	H/W 3	Credits 3	Marks 100

Course Outcomes:

The Learners will be able to

1. Identify the components in two component mixture and detect the functional groups.
2. Prepare the organic compounds and purify them.
3. Perform common laboratory techniques like separation, refluxing, recrystallization, vacuum filtration, and sublimation.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	L	H	H	H
CO2	H	H	M	H	H	H
CO3	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

1. Identification of components in a two-component mixture and preparation of their derivatives.
2. Preparations:
   (i) p-nitrobenzoic acid from p-nitrotoluene (Oxidation)
   (ii) Anthroquinone from Anthracene (Oxidation)
   (iii) 1,2,3,4 - tetrahydrocarbazole from Cyclohexanone (Reduction)
   (iv) Methyl orange from Sulphanilic acid
   (v) Acetyl Salicylic acid (Aspirin) from Salicylic acid (Acetylation)
   (vi) m-nitro aniline from m-dinitrobenzene (Reduction)

Reference Books:

1. S. Furniss Brain, Vogel's Textbook of Practical Organic Chemistry, Pearson Publication, 5th Edition**,** Reprint 2004.
2. N. S. Gnanapragasam & G. Ramamurthy, Organic Lab Manual (Semi-Micro Qualitative Analysis and Separation), S. Viswanathan Printers & Publishers Pvt., Ltd, Reprint 2002.

OER:

1. http://vlab.amrita.edu/?sub=2&brch=191&sim=345&cnt=1
2. https://www.brainkart.com/article/Organic-Qualitative-Analysis_38680/
3. http://amrita.olabs.edu.in/?sub=73&brch=8&sim=141&cnt=715

Continuous Assessment - 40 Marks

I C.A. - 50 Marks
II C.A. - 50 Marks
Average - 25 Marks
Performance during regular practicals - 10 Marks
Regularity in submission of observation notebook and Record - 5 Marks

CA Practical Examination - 50 Marks

Record - 5 Marks
Viva - 5 Marks
Experiment - 30 Marks
Preparation - 10 Marks
(Quality - 4 Marks, Quantity - 4 Marks, Recrystallization - 2 Marks)

Semester Practical Examination - 60 marks

Record - 10 Marks
Viva - 5 Marks
Qualitative Organic Analysis - 35 Marks
Preparation - 10 Marks
(Quality - 4 Marks, Quantity - 4 Marks, Recrystallization - 2 Marks)

SEMESTER II

PCCHH20 - PRACTICAL II: INORGANIC CHEMISTRY - I

Year: I SEM: II	Course Code PCCHH20	Title of the Course Practical II: Inorganic Chemistry – I	Course Type Practical	Course Category Core	H/W 3	Credits 3	Marks 100

Course Outcomes:

The Learners will be able to

1. Demonstrate group separation and analysis of inorganic mixtures.
2. Identify rare and common ions present in the inorganic mixtures.
3. Prepare selected inorganic complexes.
4. Estimate the metal ions present in the sample by colorimetric method.

CO	PSO					
	1	2	3	4	5	6
CO1	H	M	H	H	H	H
CO2	H	M	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

1. Semi micro qualitative analysis of mixture containing two common and two rare cations. (The following are the rare cations to be included - W, Te, Se, Ce, Zr, Be, V, Mo, Li)
2. Colorimetric Analysis using photoelectric method: Estimation of Iron, Nickel, Copper and Manganese.
3. Preparations:
   i. Potassium tris(oxalato)aluminate(III) trihydrate
   ii. Tris(thiourea)copper(I) chloride
   iii. Sodium hexanitrocobaltate(III)
   iv. Tetramminecopper(II) sulphate
   v. Sodium cuprousthiosulphate

Reference Books:

1. V. V. Ramanujam, Inorganic Semi Micro Qualitative Analysis, The National Publication, 3rd Edition, Reprint 2004.
2. G. Svehila, Vogel's Qualitative Inorganic Analysis, Pearson Publication, 7th Edition, Reprint 2012.

OER:

1. http://www.public.asu.edu/~jpbirk/index.html
2. http://amrita.olabs.edu.in/?sub=73&brch=7&sim=180&cnt=515
3. http://wwwchem.uwimona.edu.jm/lab_manuals/c21jexpt.html

Continuous Assessment - 40 Marks

I C.A. - 50 Marks
II C.A. - 50 Marks
Average - 25 Marks

Performance during regular practicals - 10 Marks

Regularity in submission of observation note-book and Record - 5 Marks

CA Practical Examination - 50 Marks

Record - 5 Marks
Viva - 5 Marks
Short Procedure - 5 Marks
Semi micro qualitative analysis (2 rare + 2 common cations) - 15 Marks
Preparation - 10 Marks
Colorimetric analysis - 10 Marks

Error Percentage for Colorimetric Estimation:

Upto 5% - 10 Marks
5 – 7% - 9 Marks
7 – 9% - 8 Marks
9 – 12% - 7 Marks
Above 12% - 5 Marks

Semester Practical Examination - 60 marks

Record - 10 Marks
Viva – Voce - 5 Marks
Short Procedure - 5 Marks
Semi micro qualitative analysis (2 rare + 2 common cations) - 20 Marks
Preparation - 10 Marks
Colorimetric analysis - 10 Marks

Error Percentage for Colorimetric Estimation:

Upto 5% - 10 Marks
5 – 7% - 9 Marks
7 – 9% - 8 Marks
9 – 12% - 7 Marks
Above 12% - 5 Marks

SEMESTER - II

PCCHI20 - PRACTICAL III: PHYSICAL CHEMISTRY - I

Year: I **SEM:** II	**Course Code** PCCHI20	**Title of the Course** Practical III: Physical Chemistry - I	**Course Type** Practical	**Course Category** Core	**H/W** 3	**Credits** 3	**Marks** 100

Course Outcomes:

The Learners will be able to

1. Prepare the solutions of different concentrations.
2. Experiment and calculate the rate constant of ester hydrolysis and primary salt effect.
3. Determine the order and energy of activation using kinetics.
4. Construct and analyze phase diagrams, and examine the validity of Freundlich and Langmuir adsorption isotherms.
5. Determine the rate constant using polarimeter and stability constant using photo colorimeter, and develop skills in handling colorimeter and polarimeter.

CO	**PSO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	**PO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

1. Determination of rate constant and order of the reaction of iodination of acetone in the presence of acid catalyst.
2. Determination of order of the reaction of potassium iodide and potassium persulphate.
3. Determination of the strengths of the given unknown acids and their relative strength.
4. Determination of activation energy and Arrhenius parameter for the acid catalyzed hydrolysis of methyl acetate at two different temperatures.

5. Determination of rate constant of the reaction between potassium iodide and potassium persulphate and study the effect of added neutral salt on the rate constant of the reaction.
6. Determination of adsorption of oxalic acid from aqueous solutions by activated charcoal and examines the validity of Freundlich adsorption isotherm.
7. Verification of the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.
8. Construction of the phase diagram for a binary mixture to determine the eutectic temperature and composition and determination of the composition of the given mixture A and B by making use of the phase diagram - simple eutectic system.
9. *Determination of the saponification of ethyl acetate with sodium hydroxide at equal concentrations of ester and alkali.
10. Kinetics of inversion of sucrose - polarimetry.
11. *Determination of composition of ferric ions-salicylic acid by Job's method.
12. *Determination of partial molar volume of acetic acid in aqueous solution by apparent molar volume method.

*Not to be given for examination

Reference Books:

1. V. Venkateswaran, R. Veeraswamy, A. R. Kulandaivelu, Basic Principles of Practical Physical Chemistry, Sultan Chand and Sons Educational Publishers, Reprint 1995.
2. V. K. Ahluwalia, Sunita Dhingra Adarsh Gulati, College Practical Chemistry, University Press (India) Private Limited, Reprint 2008.
3. David Shoemaker, Joseph Nibler, Carl Garland, Experiments in Physical Chemistry, 7th Edition, 2003.
4. B. D. Khosla, V. C. Garg, Adarsh Gulati, Senior Practical Physical Chemistry, R. Chand and Co., Edition 2007.

OER:

1.http://vlab.amrita.edu/?sub=3&brch=208&sim=563&cnt=958

Continuous Assessment - 40 Marks

I C.A. - 50 Marks
II C.A. - 50 Marks
Average - 25Marks
Performance during regular practicals - 10 Marks
Regularity in submission of observation notebook and Record - 5 Marks

CA Practical Examination - 50 Marks

Record - 5 Marks
Viva - 5 Marks
Principle and model graph - 5 Marks
Manipulation - 15 Marks
Result - 20 Marks

Semester Practical Examination - 60 Marks

Record - 10 Marks
Viva–Voce - 5 Marks
Principle and model graph - 5 Marks

Manipulation - 20 Marks
Result - 20 Marks

1. KINETICS: (Iodination of acetone, Second order kinetics)
Error:
Upto + 0.2 - 20 Marks
>+ 0.2 to + 0.4 - 13 Marks
> + 0.4 - 7 Marks

2. PHASE DIAGRAM FOR SIMPLE EUTECTIC SYSTEM:
Eutectic temperature and composition - 20 Marks
Eutectic temperature - 10 Marks
Error:
Upto + 2°C - 10 Marks
>+ 2°C to + 4°C - 7 Marks
>+4°C - 5 Marks
Unknown composition - 10 Marks
Upto 5% - 10 Marks
>5-6% - 7 Marks
>6% - 5 Marks

3. ARRHENIUS:
Arrhenius parameter - 10 Marks
Error:
< 1% - 10 Marks
>1-2% - 7 Marks
> 2% - 5 Marks
Activation Energy - 10 Marks
Below a factor of 10 - 10 Marks
By a factor of 10 - 7 Marks
Above a factor of 10 - 5 Marks

4. PRIMARY SALT EFFECT: (Absence of electrolyte = 10 Marks; Presence =10 Marks)
Error:
Below a factor of 10 - 10 Marks
By a factor of 10 - 7 Marks
Above a factor of 10 - 5 Marks

5. ACID STRENGTH:
Error:
< 2% - 20 Marks
>2-3% - 13 Marks
> 3% - 7 Marks

6. ADSORPTION OF ACETIC ACID/OXALIC ACID ON CHARCOAL:
Error:
< 2% - 20 Marks
>2-3% - 13 Marks
> 3% - 7 Marks

SEMESTER II

PICHC20 - IEP - CSIR-NET PREPARATORY COURSE IN INORGANIC CHEMISTRY

Year: I **SEM:** II	**Course Code** PICHC20	**Title of the Course** CSIR-NET Preparatory Course in Inorganic Chemistry	**Course Type** Theory	**Course Category** Independent Elective	**H/W** Own Pace	**Credits** 2	**Marks** 100

Learning Objective:

- Upon studying this paper, the students will be able to answer CSIR-NET questions in Inorganic Chemistry.

Course Outcomes:

The Learner will be able to

1. Apply and analyze the periodicity of properties of elements, MOT, VSEPR theory, concepts of acids and bases, and the basic aspects of solid-state chemistry.
2. Apply and analyze the properties of main group elements and their compounds.
3. Apply VB, CF and MO theories, and analyze the reactions and properties of complexes.
4. Apply and analyze the chemistry of organometallic and bioinorganic compounds.
5. Apply and analyze the various techniques involved in the characterization of inorganic compounds.

CO	**PSO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	**PO**					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I

1.1 Chemical periodicity: Periodic table, grouping of elements, classification of elements - s, p, d and f block elements, periodic trends - atomic size, ionic size, ionization potential, electronegativity. (K1, K2 & K3)

1.2 Structure and bonding: Molecular Orbital Theory - bonding and anti-bonding molecular orbitals, bond order, bonding in homo and hetero nuclear molecules. (K1, K2 & K3)

1.3 VSEPR theory: Geometries of molecules. (K1, K2, K3 & K4)

1.4 Acids and bases: Concepts of acids and bases - Arrhenius, Bronsted-Lowry and Lewis concepts, Hard-Soft Acid Base concept - Pearson theory, non-aqueous solvents. (K1, K2, K3 & K4)

1.5 Solids: Crystal systems and lattices, Miller planes, crystal packing, crystal defects, Bragg's law, ionic crystals, structures of AX, AX2, ABX3 type compounds. (K1, K2 & K3)

1.6 Spinels, band theory, metals, and semiconductors. (K1, K2, K3 & K4)

Unit II

2.1 Main group elements: General characteristics of alkali metals, alkaline earth metals, boron family, carbon family, nitrogen family, chalcogens. (K1, K2 & K3)

2.2 Compounds of main group elements - hydrides, halides, oxides, oxoacids, nitrides, sulphides - shapes and reactivity. (K1, K2 & K3)

2.3 Structure and bonding of boranes, carboranes, silicones, silicates, boron nitride, borazine and phosphazenes, industrial importance of these compounds. (K1, K2, K3 & K4)

2.4 Allotropy, chemistry of noble gases, pseudo halogens and inter halogen compounds. (K1, K2 & K3)

2.5 Transition elements: General characteristics, Ti, V, Cr, Mn and Fe group elements. (K1, K2 & K3)

2.6 Inner transition elements: Spectral and magnetic properties, redox chemistry, analytical applications. (K1, K2, K3 & K4)

Unit III

3.1 Coordination chemistry - isomerism, Valence Bond Theory (VBT). (K1 & K2)

3.2 Crystal Field Theory - energy level diagrams in various crystal fields, CFSE, applications of CFT, Jahn-Teller distortion. (K1, K2 & K3)

3.3 MOT - evidences, σ & π - bonding in complexes - construction of molecular orbital diagrams. (K1, K2 & K3)

3.4 Electronic spectra of transition metal complexes: spectroscopic term symbols, selection rules, Orgel diagrams, charge-transfer spectra. (K1, K2 & K3)

3.5 Spectral and magnetic properties of transition metal complexes. (K1, K2 & K3)

3.6 Reaction mechanisms: kinetic and thermodynamic stability, substitution reactions. (K1, K2 & K3)

Unit IV

4.1 Organometallic compounds: Synthesis, bonding and structure, and reactivity. Cages and metal clusters. (K1, K2 & K3)

4.2 18-Electron rule: Metal-alkyl, metal-carbonyl, metal-olefin and metal-carbene complexes and metallocenes. Fluxionality in organometallic complexes. (K1, K2, K3 & K4)

4.3 Types of organometallic reactions: Homogeneous catalysis - hydrogenation, hydroformylation, acetic acid synthesis, metathesis and olefin oxidation. (K1, K2 & K3)

4.4 Heterogeneous catalysis - Fischer-Tropsch reaction, Ziegler-Natta polymerization. (K1, K2 & K3)

4.5 Bioinorganic chemistry: Photosystems, porphyrins, metallo enzymes, oxygen transport, nitrogen fixation, metal complexes in medicine. (K1, K2 & K3)

4.6 Electron-transfer reactions - ISM and OSM, electron transfer in biological systems. (K1, K2, K3 & K4)

Unit V

5.1 Characterization of inorganic compounds: By IR, Raman, UV-Vis and MS. (K1, K2, K3 & K4)

5.2 Characterization of inorganic compounds: By NMR, EPR, Mössbauer and NQR. (K1, K2, K3 & K4)

5.3 Microscopic techniques - optical, electron and scanning probe techniques. (K1, K2 & K3)

5.4 Electro analytical methods - polarography, cyclic voltammetry, ion-selective electrodes. Thermo analytical methods. (K1, K2, K3 & K4)

5.5 Nuclear chemistry: Radioactivity - decay processes, half-life of radioactive elements, nuclear reactions, fission and fusion. (K1, K2 & K3)

5.6 Radio-analytical techniques and activation analysis. (K1, K2 & K3)

References Books:

1. P. S. Kalsi, J. P. Kalsi, and Ashu Chaudhary, Bioinorganic and Supramolecular Chemistry, New Age International Publishers, 4th Edition, 2020.
2. H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International Publishers, 4th Revised Edition, 2011.
3. H. J. Arnikar, Nuclear Chemistry through Problems, New Age International Publishers, 2nd Edition, 2016.
4. R. C. Mehrotra, A. Singh, Organometallic Chemistry: A Unified Approach, New Age International Publishers, Revised 2nd Edition, 1991.
5. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age International (P) Limited, Publishers, Reprint 2005.
6. W. U. Malik & *et al*, Selected Topics in Inorganic Chemistry, S. Chand, Revised Edition, 2010.
7. R. Gupta, CSIR-UGC NET: Chemical Sciences Previous Papers (Solved), RPH Editorial Board, 2014.
8. J. D. Lee, Concise Inorganic Chemistry, Wiley, Fifth Edition, 2008.
9. James E Huheey & *et al*., Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Publications, 4th Edition, 2006.
10. G. Svehla, B. Sivasankar, Vogel's Qualitative Inorganic Analysis, Pearson Publications, 7th Edition, 2012.
11. Weller, Overton, Rourke & Armstrong, Inorganic Chemistry, Oxford University Press, 6th Edition, 2015.
12. D. N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, I. K. International Publishing House Pvt. Ltd., 2nd Edition, 2013.

OER:

1. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-03, P-07, P-11 & P-15)
2. https://nptel.ac.in/course.html
3. https://www.khanacademy.org/science/chemistry

SEMESTER III

PCCHJ20 - SYNTHETIC ORGANIC CHEMISTRY

Year: II SEM: III	Course Code PCCHJ20	Title of the Course Synthetic Organic Chemistry	Course Type Theory	Course Category Core	H/W 4	Credits 4	Marks 100

Learning Objectives:

- To understand the importance of different organic reagents in organic synthesis.
- To get exposed to the mechanisms of retro synthesis and their applications.
- To learn methods of asymmetric synthesis and resolution, transition metal catalyzed reactions, chemoselectivity, regioselectivity, stereoselectivity and diastereoselectivity.

Course Outcomes:

The Learners will be able to

1. Analyze and evaluate the concepts of retrosynthesis, disconnection approach and protection of common functional groups and apply them in synthesizing target molecules.
2. Evaluate the methods of asymmetric synthesis and resolution.
3. Analyze the preparation and uses of selected organic reagents.
4. Evaluate the role of PTC in organic synthesis.
5. Appraise the role of transition metals in selected named reactions and plan chemo selective, regioselective and stereoselective named reactions.

CO	PSO					
	1	2	3	4	5	6
CO1	H	M	L	H	H	H
CO2	H	M	L	H	H	H
CO3	H	M	L	H	H	H
CO4	H	M	L	H	H	H
CO5	H	M	L	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H–High (3), M-Moderate (2), L- Low (1)

Unit I **(12 Hours)**

1.1 Retrosynthesis, disconnection approach, synthons, linear and convergent synthesis. (K1, K2, K3, K4, K5 & K6)

1.2 One group C-X disconnection and two group C-X disconnection. (K1, K2, K3, K4, K5 & K6)

1.3 Umpolung of reactivity, protection of functional groups (hydroxyl, amino, carbonyl and carboxyl groups). (K1, K2, K3, K4, K5 & K6)

1.4 Synthesis of target molecules based on disconnection and synthon approach - asprin, 3-methyl-1-pentene, methyl-3-phenyl butanoate. (K1, K2, K3, K4, K5 & K6)

1.5 Synthesis of target molecules based on disconnection and synthon approach - cis-1-isopropyl-2-benzyl ethylene and 2,6-dibromoaniline. (K1, K2, K3, K4, K5 & K6)

1.6 Synthesis of target molecules based on disconnection and synthon approach - reserpine, saccharine, paracetamol, morpholine. (K1, K2, K3, K4, K5 & K6)

Unit II **(12 Hours)**

2.1 Prostereoisomerism - prochirality, topicity of ligands and faces - homotopic. (K1, K2, K3, K4 & K5)

2.2 Heterotopic and enantiotopic ligands. (K1, K2, K3, K4 & K5)

2.3 Asymmetric synthesis, chiral auxiliaries, methods of asymmetric induction, substrate, reagent, and catalyst-controlled reactions - examples. (K1, K2, K3, K4 & K5)

2.4 Determination of enantiomeric and diastereomeric excess. (K1, K2, K3, K4 & K5)

2.5 Methods of resolution - mechanical separation, formation of diastereomers. (K1, K2, K3, K4 & K5)

2.6 Methods of resolution - chromatography and biochemical transformation. (K1, K2, K3, K4 & K5)

Unit III **(12 Hours)**

3.1 Organolithium compounds - preparation, reactions and uses (resemblance with Grignard reagent, difference from Grignard reagent). (K1, K2, K3, K4, K5 & K6)

3.2 Organosilanes - synthetic applications of trimethyl silyl iodide, trimethyl silyl chloride, trimethyl silyl cyanide and trimethyl silyl triflate. (K1, K2, K3, K4, K5 & K6)

3.3 Uses of the following reagents - DCC, 1,3-dithiane (Umpolung), Lithium diisopropylamide (LDA). (K1, K2, K3, K4, K5 & K6)

3.4 Uses of the following reagents - Diisobutylaluminium hydride (DIBAL), 9-borabicyclo[3.3.1]nonane] (9BBN), Gilman's reagent. (K1, K2, K3, K4, K5 & K6)

3.5 Preparation and uses of phosphorous ylides. (K1, K2, K3, K4, K5 & K6)

3.6 Preparation and uses of nitrogen and sulphur ylides. (K1, K2, K3, K4, K5 & K6)

Unit IV **(12 Hours)**

4.1 Principles and synthetic process involving phase transfer catalysis - nitriles from alkyl halides, benzoyl cyanides from benzoyl chlorides. (K1, K2, K3, K4 & K5)

4.2 Preparation of alkyl fluorides from alkyl halides, alcohols from alkyl halides using PTC. (K1, K2, K3, K4 & K5)

4.3 Preparation of azides from alkyl halides, sodium alkyl sulphonates from alkyl halides using PTC. (K1, K2, K3, K4 & K5)

4.4 Preparation of alkyl nitrates, thiocyanates, cyanates and p-toluenesulphonates from alkyl halides using PTC. (K1, K2, K3, K4 & K5)

4.5 Preparation of aryl ethers and thioethers, esterification using PTC. (K1, K2, K3, K4 & K5)

4.6 Diazotransfer by phase transfer catalyst, dihalocarbenes. (K1, K2, K3, K4 & K5)

Unit V **(12 Hours)**

5.1 Transition metal catalyzed reactions - reaction and mechanism of Heck reaction and Suzuki cross coupling reaction. (K1, K2, K3, K4, K5 & K6)

5.2 Reaction and mechanism of carboxymethylation, hydro formylation and epoxide-allylic alcohol rearrangement. (K1, K2, K3, K4, K5 & K6)

5.3 Chemoselectivity - reduction and oxidation - examples, calculation. (K1, K2, K3, K4, K5 & K6)

5.4 Regioselectivity - Birch reduction. (K1, K2, K3, K4, K5 & K6)

5.5 Stereoselectivity - stereoselective Claisen reaction. (K1, K2, K3, K4, K5 & K6)

5.6 Diastereoselective reaction - hydroboration (formation of an alcohol). (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. Stuart Warren, Organic Synthesis: The Disconnection Approach, Wiley Student Edition, Reprint 2007.
2. Puneet Karnad, Organic Synthesis, RBSA Publishers, 2007.
3. V. K. Ahluwalia, Organic Synthesis: Special Techniques, Narosa Publishing House, 2nd Edition, 2005.
4. S. N. Sanyal., Reactions, Rearrangements and reagents, Bharati Bhawan, Reprint 2003.
5. P. S. Kalsi, Stereo Chemistry, Conformations and Mechanisms, New Age International Pvt. Ltd., 10th Edition, 2019.
6. P. S. Kalsi, Organic Reactions and Their Mechanisms, New Age International Ltd., Reprint, 2017.
7. S. M. Mukherji and S. P. Singh, Organic Reaction Mechanism, Trinity Press, Revised Edition, 2017.
8. O. P. Agarwal, Organic Chemistry, Reactions and Reagents, 55th Edition, GOEL Publishing House, 2017.
9. W. Carruthers, Some Modern Methods of Organic Synthesis, Cambridge University Press, 4th Edition, Reprint 2004.
10. Jonathan Clayden, Nick Greeves and Stuart Warren, Organic Chemistry, Oxford University Press, 2nd Edition, 2012.
11. Francis A. Carey and Richard J, Advanced Organic Chemistry, Part B - Sundberg, 4th Edition, Reprint 2001.
12. J. March, Advanced Organic Chemistry, Wiley Inter Science, 4th Edition, Reprint 2001
13. R. K. Mackie and D. M. Smith, Guide book to Organic Synthesis, Longman Publication, Reprint 1990.
14. R. O. C. Norman, Principles of Organic Synthesis, Chapman and Hall, London, 2nd Edition, Reprint 1980.
15. E. S. Gould, Structure and Mechanism, Copyright, 1959.

OER:

1. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P014-Retrosynthesis, disconnection approach)
2. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P01-Prochirality, asymmetric synthesis)
3. Infowledge - https://www.youtube.com/watch?v=sJnqi3bQlxw (Topicity problems)
4. Infowledge - https://www.youtube.com/watch?v=0gJdVbCqf8o(Regioselectiveand chemoselective reactions)
5. Infowledge - https://www.youtube.com/watch?v=u3PCt-MNTfo(Stereoselective reactions)
6. Infowledge - https://www.youtube.com/watch?v=JLFdKFMit0Y (Enantioselective and diastereoselective reactions)

SEMESTER III

PCCHK20 - MOLECULAR SPECTROSCOPY

Year: II SEM: III	Course Code PCCHK20	Title of the Course Molecular Spectroscopy	Course Type Theory	Course Category Core	H/W 5	Credits 4	Marks 100

Learning Objectives:

- To understand the concepts of spectral techniques and to apply these techniques for the quantitative and structural analysis of organic and inorganic compounds.
- To work out combined spectroscopic problems.

Course Outcomes:

The Learners will be able to

1. Apply Ultraviolet spectroscopy for the identification of organic compounds and inorganic complexes, and to interpret the IR spectra of organic compounds and inorganic complexes.
2. Discuss the different ionization techniques involved in Mass spectroscopy, principle of GC-MS and its advantages over MS, and to elucidate the molecular formulae and structures of unknown compounds using Mass spectroscopy.
3. Analyze the splitting pattern in the ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR spectra for structural determination. Discuss the principle, instrumentation and applications of Mossbauer spectroscopy and analyze the Mossbauer spectra of iron and tin compounds.
4. Explain hyper fine splitting in EPR and interpret EPR spectra of simple radicals and complexes, and to explain the electronic spectra for chemical analysis.
5. Elaborate on the concepts and theories of microwave, IR, rotational and vibrational Raman, and electronic spectroscopy.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Ultra violet spectroscopy - Woodward-Fieser rules for conjugated dienes, polyenes and alpha, beta unsaturated carbonyl compounds. The effect of steric hindrance to coplanarity - charge transfer spectral absorption. (K1, K2, K3, K4, K5 & K6)

1.2 Transitions in transition metal complexes - selection rules for electronic transitions - band widths - nature of electronic transitions in complexes. Auxochrome - types - chromophore concept - types. (K1, K2, K3, K4, K5 & K6)

1.3 Applications of UV Spectroscopy. (K1, K2, K3, K4, K5 & K6)

1.4 Applications of IR spectroscopy to identify alkane, alkene, alkyne, aromatic compounds, nitrile and aromatic residues. Identification of alcohols, ethers, phenols, amines and carbonyl compounds such as ketones, aldehydes, esters, amides, acids, hetero aromatic compounds, halogen compounds, sulphur compounds, thiocyanates and isothiocyanates, amino acids and amines. (K1, K2, K3, K4, K5 & K6)

1.5 Metal-ligand stretching vibrations for metal carbonyls, sulphates, thiocyanides, nitro and nitrito complexes. (K1, K2, K3, K4, K5 & K6)

1.6 Applications of IR Spectroscopy - quantitative analysis, qualitative analysis, coordination compounds, hydrogen bonding studies, calculation of force constants and determination of aromaticity. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Mass spectroscopy - ionization techniques such as chemical ionization, electron ionization - ESI, FD, FAB, SIMS and MALDI. (K1, K2, K3, K4 & K5)

2.2 Molecular ions, isotope ions, meta-stable peak, secondary ion mass spectroscopy. nitrogen rule and ring rule, fragment ions of odd and even electron types. (K1, K2, K3, K4 & K5)

2.3 Rearrangement ions - cleavage patterns - simple and multi center fragmentation. (K1, K2, K3, K4 & K5)

2.4 Applications of mass spectra to elucidate molecular formula and structure. (K1, K2, K3, K4 & K5)

2.5 McLafferty rearrangement - interpretation of fragmentation pattern of phenols, aldehydes, lactones, nitro compounds, esters, acetals and ketals, hetero aromatic compounds, and sulphides. (K1, K2, K3, K4 & K5)

2.6 Introduction to GC-MS and its advantages over MS. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 NMR spectroscopy - introduction - nuclear spin - Larmor frequency, precessional frequency - relaxation process - chemical shift - shielding constants - ring current and aromaticity - shifts for ^{1}H and ^{13}C. (K1, K2, K3, K4, K5 & K6)

3.2 Spin-spin interaction - nuclear magnetic double resonance - Nuclear Overhauser Effect (NOE). (K1, K2, K3, K4, K5 & K6)

3.3 Applications of $^{1}HNMR$, $^{13}CNMR$, $^{31}PNMR$ (HPF_2, H_3PO_2, H_3PO_3, H_3PO_4 and P_4S_3), $^{19}FNMR$ (ClF_3, ClF_5, SF_4 and BrF_5) and their applications to inorganic systems. (K1, K2, K3, K4, K5 & K6)

3.4 Mossbauer spectroscopy - Mossbauer effect - recoilless emission and absorption, Doppler effect, hyperfine interaction - chemical isomer shift, quadruple interaction, and magnetic splitting. (K1, K2, K3, K4, K5 & K6)

3.5 Instrumentation - selection of suitable source, limitations. (K1, K2, K3, K4, K5 & K6)

3.6 Interpretation of spectra - bonding and structures of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds and detection of oxidation states and in-equivalent MB atoms, applications of Mossbauer spectroscopy. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 ESR - principle, origin of an EPR signal, derivative spectra, g value - factors affecting the magnitude of g values, anisotropy, hyperfine splitting - hyperfine coupling constant, relative intensities of EPR signals. (K1, K2, K3, K4 & K5)

4.2 Interpretation of the spectra of simple carbon centered free radicals, hyperfine splitting in Cu and Mn compounds, zero field splitting and Kramer's degeneracy. (K1, K2, K3, K4 & K5)

4.3 Electron delocalization - Mc Connell's equation, line width in solid state EPR, applications of ESR. (K1, K2, K3, K4 & K5)

4.4 Photoelectron spectroscopy - photo electric effect, UV and X-ray PES, Koopmans' theorem, fine structure in PES. (K1, K2, K3, K4 & K5)

4.5 Interpretation of photo electron spectra of H_2, N_2, O_2, CO, NO, N_2O, H_2O, azide, HCl and NH_3. (K1, K2, K3, K4 & K5)

4.6 Electron Spectroscopy for Chemical Analysis - applications of ESCA. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Rotational spectroscopy: Classification of molecules, molecular energy levels, the rigid rotator, selection rules, intensity of spectral lines, effect of isotopic substitution. (K1, K2, K3, K4, K5 & K6)

5.2 Non rigid rotator, microwave spectra of polyatomic molecules. (K1, K2, K3, K4, K5 & K6)

5.3 Vibrational spectroscopy: Vibrational energy of diatomic molecules, simple harmonic oscillator, selection rules, zero-point energy, force constant and bond strength. (K1, K2, K3, K4, K5 & K6)

5.4 Anharmonicity, Morse potential energy diagram, Franck Condon principle, the diatomic vibrating rotator, P, Q, R, branches, the vibration-rotation spectrum of CO. (K1, K2, K3, K4, K5 & K6)

5.5 Breakdown of Born-Oppenheimer approximation, vibrations of polyatomic molecules, normal modes of vibration, overtones, hot bands, Fermi resonance. (K1, K2, K3, K4, K5 & K6)

5.6 Raman: Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, stokes and anti-stokes lines, mutual exclusion principle. (K1, K2, K3, K4, K5 & K6)

Combined spectroscopic problems (organic and inorganic compounds)

Reference Books:

1. J. Dyer, Application of Absorption Spectroscopy of Organic Compounds, Prentice Hall of India Pvt. Ltd., New Delhi, 2005.
2. R. M. Silverstein, G. D. Bassler and Monsu, Spectrometric Identification of Organic Compounds, John Wiley and Sons, New York, 6th Edition, 2005.
3. I. L. Finar, Organic Chemistry, Vol. II, ELBS Publication, 5th Edition, 2005.
4. P.S. Kalsi, Spectroscopy of Organic Compounds, New Age International (P) Limited, 6th Edition, 2007.

5. B. K. Sharma, Spectroscopy, Goel Publishing House, Delhi, 2019.
6. Dr. H. Kaur, Spectroscopy, Pragati Prakashan, Meerut, 14th Edition, 2018.
7. William Kemp, Organic Spectroscopy, Palgrave Publishers Ltd, New York, Reprint 2017.
8. L. D. S. Yadav, Organic Spectroscopy, Kluwer Academic Publishers, 2005.
9. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, Introduction to Spectroscopy, Brooks/Cole, Cengage Learning, 2009.
10. Y. R. Sharma, Elementary Organic Spectroscopy: Principles and Chemical Applications, S. Chand & Company Pvt. Ltd., 2013.
11. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, Blackwell Scientific Publishers, 1986.
12. R. S. Drago, Physical Methods in Inorganic Chemistry, Wiley Eastern Company, 3rd Edition, 1972.
13. G. R. Chatwal and S. K. Anand, Spectroscopy: Atomic and Molecular, Himalaya Publishing House, 2016.
14. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, 4th Edition, 2017.
15. D. N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International Publishers, 2015.
16. K. V. Raman, R. Gopalan, P. S. Raghavan, Molecular Spectroscopy, Thomson Publication, Copyright 2004.
17. G. Aruldhas, Molecular Structure and Spectroscopy, PHI Learning, 2nd Edition, 2009.

OER:

1. https://nptel.ac.in/courses/104/106/104106122/ (Introduction to spectroscopy)
2. http://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (Woodward-Fieser rules)
3. http://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5

   (Mass-General fragmentation rules)
4. https://nptel.ac.in/courses/104/106/104106048/ (ESR Spectroscopy)
5. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5

(P-08-Physical Spectroscopy)

SEMESTER III

PCCHL20 - ELECTRO CHEMISTRY

Year: II SEM: III	Course Code PCCHL20	Title of the Course Electro Chemistry	Course Type Theory	Course Category Core	H/W 4	Credits 4	Marks 100

Learning Objectives:

- To have an in-depth knowledge on the theory of strong electrolytes.
- To learn the principles and techniques involved in polarography, cyclic voltammetry, amperometric and potentiometric titrations.
- To gain knowledge regarding electrode-electrolytic interface.
- To study the principle and functioning of fuel cells and electrochemical sensors.

Course Outcomes:

The Learners will be able to

1. Examine the concepts and theories of strong electrolytes and verify the Debye Huckle Onsager equation.
2. Explain the principle and application of various analytical techniques.
3. Compare the structure of double layers.
4. Examine and predict the kinetics of electrode reaction of single step and multistep and discuss the theories and mechanism of corrosion and passivation.
5. Classify the types of fuel cells and ion selective electrodes.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(12 Hours)**

1.1 Activity and activity coefficients, mean ionic activity and mean ionic activity coefficient, concept of ionic strength, related problems. (K1, K2, K3, K4, K5 & K6)

1.2 Debye Huckel theory of strong electrolytes - electrolytic conductance - interionic attraction - ionic atmosphere. (K1, K2, K3, K4, K5 & K6)

1.3 Determination of activity coefficient by electro chemical method. (K1, K2, K3, K4, K5 & K6)

1.4 Derivation of Debye Huckel limiting law, qualitative and quantitative verification. (K1, K2, K3, K4, K5 & K6)

1.5 Debye Huckel limiting law at appreciable concentrations of electrolytes. (K1, K2, K3, K4, K5 & K6)

1.6 Derivation of Debye Huckel Onsager equation - experimental verification and limitations. (K1, K2, K3, K4, K5 & K6)

Unit II **(12 Hours)**

2.1 Polarography - theory, apparatus, DME, diffusion, kinetic and catalytic currents, current for reversible and irreversible systems, qualitative and quantitative application to inorganic systems. (K1, K2, K3, K4 & K5)

2.2 Amperometric titrations - theory, apparatus, types of titration curves, applications. (K1, K2, K3, K4 & K5)

2.3 Biamperometric titrations - successive titrations, indicator electrodes, applications. (K1, K2, K3, K4 & K5)

2.4 Cyclic Voltammetry - theory, instrumentation, application to inorganic systems. (K1, K2, K3, K4 & K5)

2.5 Potentiometry - potentiometric titrations, equivalence point potential for Fe^{2+}/Fe^{3+}-MnO_4^-, H^+/Mn^{2+} systems. (K1, K2, K3, K4 & K5)

2.6 Potentiometric titrations - determination of concentration of the species at the equivalence point. (K1, K2, K3, K4 & K5)

Unit III **(12 Hours)**

3.1 Electrode-electrolyte interface, adsorption at electrified interface, electrical double layer. (K1, K2, K3, K4, K5 & K6)

3.2 Electro capillary phenomenon - Lippmann equation. (K1, K2, K3, K4, K5 & K6)

3.3 Structure of double layers - Helmholtz Perrin, Gouy-Chapman, and Stern model of electrical double layers. (K1, K2, K3, K4, K5 & K6)

3.4 Diffusion - Fick's law of diffusion - factors affecting Fick's law of diffusion - significance. (K1, K2, K3, K4, K5 & K6)

3.5 Membrane potential - current across the biological membrane - axon membrane. (K1, K2, K3, K4, K5 & K6)

3.6 Electrokinetic phenomena - electroosmosis, electrophoresis, sedimentation potential and streaming potential. (K1, K2, K3, K4, K5 & K6)

Unit IV **(12 Hours)**

4.1 Over potential - mechanism of the hydrogen and oxygen evolution reaction. Rates of simple electrode reactions - elementary electron - electrode process. (K1, K2, K3, K4 & K5)

4.2 Butler-Volmer equation for single step electron transfer reaction, significance of electron exchange current density and symmetry factor. (K1, K2, K3, K4 & K5)

4.3 Rates of multistep electrode reactions, Butler-Volmer equation for a multistep reaction, transfer coefficient and its significance. (K1, K2, K3, K4 & K5)

4.4 Corrosion of metals - theories of corrosion - types of corrosion - Pourbaix diagram (K1, K2, K3, K4 & K5)

4.5 Passivation of metals - Flade Potential - Evan's diagram (K1, K2, K3, K4 & K5)

4.6 Electro deposition - principle and applications, electrochemical reactions of technological interest. (K1, K2, K3, K4 & K5)

Unit V **(12 Hours)**

5.1 Fuel cells - efficiency, types of fuel cells - alkaline fuel cell, phosphoric acid, high temperature and solid polymer electrolyte. (K1, K2, K3, K4, K5 & K6)

5.2 Kinetics of fuel cell, general development of fuel cell technology. (K1, K2, K3, K4, K5 & K6)

5.3 Electrochemical sensors - ion selective electrodes - problems with ion selective electrodes. (K1, K2, K3, K4, K5 & K6)

5.4 Chemically modified electrodes - gas sensing electrodes. (K1, K2, K3, K4, K5 & K6)

5.5 Principle and working of enzyme electrodes. (K1, K2, K3, K4, K5 & K6)

5.6 Sensors based on modified metal-oxide-semiconductor field-effect transistors (MOSFET) - wall jet ring disc electrodes (WJRDE). (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. S. Glasstone, Introduction to Electro Chemistry, Affiliated East West Press, New Delhi, 1960.
2. J. O. M. Bockris and A. K. N. Reddy, Electro Chemistry - Volumes 1 and 2, Plenum, New York, 1977.
3. Willard, Merritt, Dean and Settle, Instrumental Methods of Analysis, CBS Publications, New Delhi, 6th Edition, 1986.
4. D. A. Skoog, Principles of Instrumental Methods of Analysis, Saunders College Publication, 3rd Edition, 1985.
5. G. D. Christian and J. E. G. Reily, Allegn Becon, Instrumental Analysis, 2nd Edition, 1986.
6. M. S. Yadav, Instrumental Methods of Chemical Analysis, Campus Books International, 2006.
7. B. Viswanathan and M. Aulice Scibioh, Fuel Cells: Principles and Applications, Reprint 2009.

OER:

1. https://ocw.mit.edu/courses/chemical-engineering/10-626-electrochemical-energy-systems-spring-2014/lecture-notes/
2. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Supplemental_Modules_(Analytical_Chemistry)/Analytical_Sciences_Digital_Library/Active_Learning/In_Class_Activities/Electrochemical_Methods_of_Analysis/02_Text/7%3A_Electrochemical_Analytical_Methods/7.4%3A_Titrimetic_Methods_of_Analysis
3. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Supplemental_Modules_(Analytical_Chemistry)/Analytical_Sciences_Digital_Library/JASDL/Courseware/

Analytical_Electrochemistry%3A_The_Basic_Concepts/03_Fundamentals_of_Electrochemistry/A._Electrochemical_Thermodynamics/02_Electrical_Double_Layer_and_Charging_Current

4. https://americanhistory.si.edu/fuelcells/index.html
5. https://chem.libretexts.org/Bookshelves/Analytical_Chemistry/Supplemental_Modules_(Analytical_Chemistry)/Analytical_Sciences_Digital_Library/JASDL/Courseware/Analytical_Electrochemistry%3A_Potentiometry/03_Potentiometric_Theory/03_Ion-Selective_Electrodes

SEMESTER III

PECHE20 - ELECTIVE III A: ANALYTICAL CHEMISTRY

Year: II SEM: III	Course Code PECHE20	Title of the Course Analytical Chemistry	Course Type Theory	Course Category Core Elective	H/W 5	Credits 5	Marks 100

Learning Objectives:

- To study in detail the different types of chromatographic techniques and their applications.
- To give an in-depth knowledge on environmental chemistry and its impacts.
- To understand the applications of computers in chemistry.

Course Outcomes:

The Learners will be able to

1. Compare different thermal methods of analysis and explain their applications in material science.
2. Elaborate the principle, instrumentations of the Gas, HPLC and SCF chromatographic techniques and their applications.
3. Examine the identification of metal ions using AAS and photo acoustic spectroscopy.
4. Solve simple problems in chemistry using 'C' program.
5. Analyze the importance of Green Chemistry and its impact on the sustainable environment and the quality of water.

CO	PSO					
	1	2	3	4	5	6
CO1	H	M	L	H	H	H
CO2	H	M	L	H	H	H
CO3	H	M	L	H	H	H
CO4	H	M	L	H	H	H
CO5	H	M	L	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Thermal Analysis - Thermo Gravimetric Analysis (TGA) - principle, instrumentation, thermogravimetric curves of $CaC_2O_4.H_2O$, $MgCr_2O_4$, Hg_2CrO_4, Ag_2CrO_4, $AgNO_3$ and $Cu(NO_3)_2$. (K1, K2, K3, K4, K5 & K6)

1.2 Factors affecting TGA, applications of TGA. (K1, K2, K3, K4, K5 & K6)

1.3 DTG - principles, comparison of DTG & TGA. (K1, K2, K3, K4, K5 & K6)

1.4 Differential Thermal Analysis (DTA) - principle, instrumentation, simultaneous TGA and DTA curves and applications. (K1, K2, K3, K4, K5 & K6)

1.5 Differential Scanning Calorimetry (DSC) - principle, instrumentation and applications. (K1, K2, K3, K4, K5 & K6)

1.6 Thermometric titrations - principle, instrumentation and applications. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Chromatographic techniques: Gas Chromatography, principle, types, instrumentation with block diagram - carrier gas, sample injection system, column, thermal compartment, detectors, recorder. (K1, K2, K3, K4 & K5)

2.2 Applications of GC. ((K1, K2, K3, K4 & K5)

2.3 High Pressure Liquid Chromatography (HPLC) - principle, characteristics of HPLC. (K1, K2, K3, K4 & K5)

2.4 Instrumentation, applications, comparison of HPLC with GLC. (K1, K2, K3, K4 & K5)

2.5 Super Critical Fluid Chromatography (SCFC) - principle, properties, instrumentation. (K1, K2, K3, K4 & K5)

2.6 Comparison with other types of chromatography, super critical fluid extraction and applications. (K1, K2, K3, K4 & K5)\

Unit III **(15 Hours)**

1.1 Atomic absorption spectrometry - principle, difference between AAS and AES, measurement of absorption. (K1, K2, K3, K4, K5 & K6)

1.2 Instrumentation with block diagram - radiation source, atomization unit, oxidizing agents, flame and non-flame atomizer, burners, monochromators, detectors, and amplifier and readout devices. (K1, K2, K3, K4, K5 & K6)

1.3 Interferences in AAS - spectral, chemical, ionization, dissociation of metal compounds, effect of solvent. (K1, K2, K3, K4, K5 & K6)

1.4 Differences between atomic absorption and emission methods, advantages and disadvantages of atomic emission spectroscopy, advantages of AAS over flame emission spectroscopy, disadvantages of AAS. (K1, K2, K3, K4, K5 & K6)

1.5 Applications of AAS, some typical analysis like determination of metals like Na, K, Ca and Mg in blood serum, lead in petrol, metals in food stuff. (K1, K2, K3, K4, K5 & K6)

1.6 Photo acoustic spectroscopy: Principle, instrumentation with block diagram and applications. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Computers in Chemistry - introduction to computers - types of computers, hardware, software, types of software and programming languages - implementation and uses. (K1, K2, K3, K4 & K5)

4.2 C-Programming - definition, types of variables with examples, constant - definition, types with examples, C-operators - classification with examples. (K1, K2, K3, K4 & K5)

4.3 Input and output functions, control statement, loop, go to statement - functions, arrays and pointers. (K1, K2, K3, K4 & K5)

4.4 Calculation of pH, solubility product, calculation of bond energy using Born-Lande equation. (K1, K2, K3, K4 & K5)

4.5 Internet: Introduction to internet service providers in India, terms used in internet, www, http, html, TCP/IP band width, dialup service. (K1, K2, K3, K4 & K5)

4.6 ISDN and search engines. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Environmental chemistry: Water quality standards - BOD, COD, TDS, TSS & TS. (K1, K2, K3, K4, K5 & K6)

5.2 Analysis of waste water and its treatment. (K1, K2, K3, K4, K5 & K6)

5.3 Salinity of water and its treatment - Reverse Osmosis. (K1, K2, K3, K4, K5 & K6)

5.4 Toxic chemicals in environment - toxicity of mercury, lead, chromium, arsenic. (K1, K2, K3, K4, K5 & K6)

5.5 Green chemistry - principle, conditions followed in green synthesis. (K1, K2, K3, K4, K5 & K6)

5.6 Carbon-carbon bond formation in aldol condensations like silyl enol ethers in aqueous media, solid phase, supercritical water and asymmetric aldol condensation. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. H. Kaur, Instrumental Methods of Chemical Analysis, Pragati Prakashan, Meerut, 3rd Edition, 2010.
2. B. K. Sharma, Instrumental Methods of Chemical Analysis, Krishna Prakashan Media (P) Ltd., 2014.
3. Y. Anjaneyulu, K. Chandrasekhar, Valli Manickam, A Textbook of Analytical Chemistry, Pharma Book Syndicate, Hyderabad, 2019.
4. V. K. Ahluwalia, Strategies for green organic synthesis, Ane Books Pvt. Ltd., New Delhi, 2012.
5. Willard Merritt, Dean Settle, Instrumental Methods of Analysis, CBS Publishers and Distributors, New Delhi, 7th Edition, 2018.
6. Skoog, Holler, Nieman, Principles of Instrumental Analysis, Thomson Books, United Kingdom, 5th Edition, 2005.
7. Skoog, West, Holler, Rouch, Fundamentals of Analytical Chemistry, Brooks/ Cole Cengage Learning, 9th Edition, 2013.
8. Jag Mohan, Organic Analytical Chemistry Theory and Practice, Narosa Publishing House, New Delhi, 2014.
9. A. K. De, Environmental Chemistry, New Age International Publishers, New Delhi, 7th Edition, 2010.

10. G. S. Sodhi, Fundamental Concept of Environmental Chemistry, Narosa Publishing House, 3rd Edition, New Delhi, 2013.
11. S. S. Dara, A Textbook of Environmental Chemistry and Pollution Control, S. Chand and Company Ltd., New Delhi, 2004.
12. S. M. Khopkar, Basic Concept of Analytical Chemistry, New Age International (P) Ltd. Publishers, New Delhi, 3rd Edition, 2008.
13. G. I. David Krupadanan, D. Vijaya Prasad, K. Varaprasad Rao, K. L. N. Reddy, C. Sudhakar, Analytical Chemistry, University Press, Hyderabad, Andhra Pradesh, 2001.
14. K. V. Raman, Computers in Chemistry, Tata McGraw-Hill, New Delhi, 2013.
15. Krishnan Kannan, Environmental Chemistry, Chand and Co. Ltd., 1995.
16. M. S. Yadav, Instrumental Methods of Chemical Analysis, Campus Books International, 2006.
17. A.K. Srivatasava, P.C. Jain, Instrumental Approach to Chemical Analysis, S. Chand & Company, 2010

OER:

1.https://www.americanpharmaceuticalreview.com/Featured-Articles/36776-Thermal-Analysis-A-Review-of-Techniques-and-Applications-in-the-Pharmaceutical-Sciences/
2.https://nptel.ac.in/content/storage2/courses/102103044/pdf/mod5.pdf
3.https://www.iitk.ac.in/che/pdf/resources/AAS-GTA-reading-material.pdf
4.https://www.epa.gov/greenchemistry/basics-green-chemistry

SEMESTER III

PECHF20 - ELECTIVE III B: GREEN CHEMISTRY

Year: II SEM: III	Course Code PECHF20	Title of the Course Green Chemistry	Course Type Theory	Course Category Core Elective	H/W 5	Credits 5	Marks 100

Learning Objectives:

- To understand the goals and principles of green chemistry.
- To explain the green reactions.
- To understand the good laboratory practices and designing of green synthesis.
- To learn selected green preparations.
- To analyze the future trends in green chemistry.

Course Outcomes:

The Learners will be able to

1. Explain the goals and progress of green chemistry.
2. Summarize the principle of green chemistry and green reactions.
3. Discuss the good laboratory practices and designing of green synthesis, and to explain the mechanism and applications of certain named reactions and rearrangements.
4. Explain selected green preparations.
5. Analyze the future trends in green chemistry.

CO	PSO					
	1	2	3	4	5	6
CO1	H	M	M	H	H	H
CO2	H	M	M	H	H	H
CO3	H	M	M	H	H	H
CO4	H	M	M	H	H	H
CO5	H	M	M	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Green chemistry - definition, need for green chemistry. (K1, K2, K3, K4, K5 & K6)

1.2 Goals of green chemistry, the roots of innovation and its limitations. (K1, K2, K3, K4, K5 & K6)

1.3 Progress of green chemistry and planning a green synthesis in a chemical laboratory. (K1, K2, K3, K4, K5 & K6)

1.4 Percentage atom utilization, atom economy. (K1, K2, K3, K4, K5 & K6)

1.5 Evaluating the type and selection of starting materials. (K1, K2, K3, K4, K5 & K6)

1.6 Biocatalysts - production of bulk and fine chemicals by microbial fermentation. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Principles of green chemistry - twelve principles of green chemistry. (K1, K2, K3, K4 & K5)

2.2 Green reactions – addition and elimination reactions. (K1, K2, K3, K4 & K5)

2.3 Green reactions - substitution reactions. (K1, K2, K3, K4 & K5)

2.4 Concept of selectivity - chemoselectivity and regioselectivity. (K1, K2, K3, K4 & K5)

2.5 Enatioselectivity and diastereoselectivity. (K1, K2, K3, K4 & K5)

2.6 Green solvents - definition and uses. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Good laboratory practices - sampling preparation for analysis. (K1. K2, K3, K4, K5 & K6)

3.2 Equipment & glass wares - selection, suitability, cleaning and drying. (K1. K2, K3, K4, K5 & K6)

3.3 Designing a green synthesis - choice of starting materials (reagents, catalysts, solvents) (K1. K2, K3, K4, K5 & K6)

3.4 Mechanism and applications of Barbier and Barton reactions. (K1. K2, K3, K4, K5 & K6)

3.5 Mechanism and applications of Cannizzaro reaction. (K1. K2, K3, K4, K5 & K6)

3.6 Mechanism and applications of Claisen rearrangement and Baker-Venkataraman rearrangements. (K1. K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Green preparations - **a**queous phase reactions (hydrolysis, iodoform). (K1, K2, K3, K4 & K5)

4.2 Solid state reactions (phenyl benzoate). (K1, K2, K3, K4 & K5)

4.3 Photochemical reactions (benzopinacol, conversion of trans-stilbene into cis-stilbene). (K1, K2, K3, K4 & K5)

4.4 PTC catalyzed reactions (phenyl isocyanide, flavone). (K1, K2, K3, K4 & K5)

4.5 Microwave assisted reactions - Hofmann elimination and esterification. (K1, K2, K3, K4 & K5)

4.6 Microwave assisted reactions – saponification, preparation of Schiff's bases. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Future trends in green chemistry - green nanosynthesis (biosynthesis of nanoparticles using plant extracts). (K1, K2, K3, K4, K5 & K6)
5.2 Green analytical methods - enzymatic transformation (ethanol, benzoin). (K1, K2, K3, K4, K5 & K6)
5.3 Green polymer chemistry - polymer from renewable resources. (K1, K2, K3, K4, K5 & K6)
5.4 Redox reagents and green catalysts. (K1, K2, K3, K4, K5 & K6)
5.5 Proliferation of solvent-less reactions and biomimetic. (K1, K2, K3, K4, K5 & K6)
5.6 Combinational green chemistry, green chemistry in sustainable developments. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. V. Kumar, Introduction to Green Chemistry, Vishal Publishing Co., 1st Edition, 2007.
2. V. K. Ahluwalia, Green Chemistry, Ane Books India, 1st Edition, 2006.
3. V. K. Ahluwalia, Agarwal K., Organic Synthesis: Special Techniques, Narosa Publishing House, 1st Edition, 2005.
4. Rashmi Sanghi, M. M. Srivastava, Green Chemistry, Alpha Science, Fourth Reprint, 2009.
5. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, Fundamentals of Analytical Chemistry, Cengage Learning, 9th Edition, 2013.

OER:

1. https://shodhganga.inflibnet.ac.in/bitstream/10603/55041/7/07_chapter%201.pdf (Introduction to green chemistry)
2. https://www.youtube.com/watch?v=J9SpYVx8H68 (Dr. Paul Anastas - Father of green chemistry)
3. https://www.youtube.com/watch?v=NycWPUcN4YI (Dr. Paul Anastas)
4. https://www.youtube.com/watch?v=v6V22gwqxeY (Dr. Paul Anastas)

Teaching and Research Aptitude – PGTRA22

Unit I – Teaching and Research Methodology

Sub Unit 1 : Teaching : Nature, objectives, characteristics and basic requirements
Sub Unit 2 : Learner's Characteristics
Sub Unit 3 : Factor's affecting teaching, methods of teaching, Teaching aids and Evaluation System
Sub Unit 4 : Research, meaning, characteristics and types
Sub Unit 5 : Steps of research and methods of research
Sub Unit 6 : Paper, article, workshop, conference and symposium, thesis writing, its Characteristics and format

Unit II – Reading Comprehension and Communication

Sub Unit 1 : Reading Comprehension
Sub Unit 2 : Passage to be set with questions to be answered
Sub Unit 3 : Communication, its nature, characteristics and objectives
Sub Unit 4 : Types and barriers of communication
Sub Unit 5 : Effective classroom communication
Sub Unit 6 : Mass media and society

Unit III – Reasoning ability and Data Interpretation
Sub Unit 1 : Number series and Letter Series
Sub Unit 2 : Codes, Relationships and Classification
Sub Unit 3 : Verbal Analogies, Inductive and Deductive Reasoning
Sub Unit 4 : Sources, acquisition and interpretation of data
Sub Unit 5 : Quantitative and Qualitative data
Sub Unit 6 : Graphical representation and mapping of data

Unit IV – Information and Communication Technology
Sub Unit 1 : General abbreviations in ICT
Sub Unit 2 : ICT – Terminologies
Sub Unit 3 : Basics of Internet and Intranet
Sub Unit 4 : Basics of E-mail – Audio and Video conferencing
Sub Unit 5 : Digital Initiatives in Higher Education
Sub Unit 6 : ICT and Governance

Unit V – People Development and Environment
Sub Unit 1 : Development and Environment
Sub Unit 2 : Human and environment interaction
Sub Unit 3 : Environmental issues
Sub Unit 4 : Natural and energy resources
Sub Unit 5 : Natural hazards and disasters
Sub Unit 6 : Environmental Protection Act and Action Plan

SEMESTER III

PICHE20 - IEP - CSIR-NET PREPARATORY COURSE IN ORGANIC CHEMISTRY

Year: II **SEM:** III	**Course Code** PICHE20	**Title of the Course** CSIR-NET Preparatory Course in Organic Chemistry	**Course Type** Theory	**Course Category** Independent Elective	**H/W** Own Pace	**Credits** 2	**Marks** 100

Learning Objective:

- To apply the theories, concepts, processes and principles of organic chemistry to qualify UGC-CSIR and other competitive examinations.

Course Outcomes:

The Learner will be able to

1. Evaluate and apply the theories, concepts, processes, and principles of stereochemistry to qualify UGC-CSIR and other competitive examinations.
2. Appraise the reaction intermediates and named reactions in organic chemistry to qualify UGC-CSIR and other competitive examinations.
3. Examine the organic transformations and asymmetric synthesis to qualify UGC-CSIR and other competitive examinations.
4. Evaluate the pericyclic reactions and applications of heterocyclic compounds to qualify UGC-CSIR and other competitive examinations.

5. Examine the natural product chemistry to qualify UGC-CSIR and other competitive examinations.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I

1.1 IUPAC nomenclature of organic molecules including regio and stereo isomers. (K1, K2, K3, K4, K5 & K6)

1.2 Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds. (K1, K2, K3, K4, K5 & K6)

1.3 Stereogenicity, stereoselectivity. (K1, K2, K3, K4, K5 & K6)

1.4 Enantioselectivity, diastereoselectivity. (K1, K2, K3, K4, K5 & K6)

1.5 Asymmetric induction. (K1, K2, K3, K4, K5 & K6)

1.6 Aromaticity: benzenoid and non-benzenoid compounds - generation and reactions. (K1, K2, K3, K4, K5 & K6)

Unit II

2.1 Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals. (K1, K2, K3, K4, K5 & K6)

2.2 Radical anions, radical cations, carbenes, benzynes and nitrenes - generation, stability and reactivity. (K1, K2, K3, K4, K5 & K6)

2.3 Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic and radical species. (K1, K2, K3, K4, K5 & K6)

2.4 Determination of reaction pathways. (K1, K2, K3, K4, K5 & K6)

2.5 Common named reactions (C-C and C=C formation). (K1, K2, K3, K4, K5 & K6)

2.6 Rearrangements (anionotropic, cationotropic, intermolecular and intramolecular) - applications in organic synthesis. (K1, K2, K3, K4, K5 & K6)

Unit III

3.1 Organic transformations and reagents: Functional group interconversion including oxidations and reductions. (K1, K2, K3, K4, K5 & K6)

3.2 Common catalysts and reagents (organic, inorganic, organometallic and enzymatic). (K1, K2, K3, K4, K5 & K6)

3.3 Chemo, regio and stereoselective transformations. (CAN, Grignard reagent, Gilmann reagent, PCC, DCC, 9BBN, BBQ and other reagents) (K1, K2, K3, K4, K5 & K6)

3.4 Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups. (K1, K2, K3, K4, K5 & K6)

3.5 Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction - substrate, reagent and catalyst-controlled reactions. (K1, K2, K3, K4, K5 & K6)

3.6 Determination of enantiomeric and diastereomeric excess, enantio-discrimination. Resolution - optical and kinetic. (K1, K2, K3, K4, K5 & K6)

Unit IV

4.1 Pericyclic reactions - electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. (K1, K2, K3, K4, K5 & K6)

4.2 Principles and applications of photochemical reactions in organic chemistry. (K1, K2, K3, K4, K5 & K6)

4.3 Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S) - oxirane, azirane. (K1, K2, K3, K4, K5 & K6)

4.4 Aziridine, thioepoxides. (K1, K2, K3, K4, K5 & K6)

4.5 Pyrrole, furan, thiophene. (K1, K2, K3, K4, K5 & K6)

4.6 Pyridine, pyran. (K1, K2, K3, K4, K5 & K6)

Unit V

5.1 Chemistry of natural products - carbohydrates. (K1, K2, K3, K4, K5 & K6)

5.2 Proteins and peptides, fatty acids. (K1, K2, K3, K4, K5 & K6)

5.3 Nucleic acids, terpenes. (K1, K2, K3, K4, K5 & K6)

5.4 Steroids and alkaloids. (K1, K2, K3, K4, K5 & K6)

5.5 Biogenesis of terpenoids and alkaloids. (K1, K2, K3, K4, K5 & K6)

5.6 Structure determination of organic compounds by IR, UV-Vis, ^{1}H and ^{13}C NMR and Mass spectroscopic techniques. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. Stuart Warren, Organic Synthesis: The Disconnection Approach, Wiley Student Edition, Reprint 2007.
2. Puneet Karnad, Organic Synthesis, RBSA Publishers, 2007.
3. V. K. Ahluwalia, Organic Synthesis: Special Techniques, Narosa Publishing House, 2nd Edition, 2005.
4. S. N. Sanyal., Reactions, Rearrangements and reagents. Bharati Bhawan, Reprint 2003.
5. P. S. Kalsi, Stereo Chemistry, Conformations and Mechanisms, New Age International Pvt. Ltd., 10th Edition, 2019.
6. P. S. Kalsi, Organic Reactions and Their Mechanisms, New Age International Ltd., Reprint, 2017.
7. S. M. Mukherji and S. P. Singh, Organic Reaction Mechanism, Trinity Press, Revised Edition, 2017.

8. O. P. Agarwal, Organic Chemistry, Reactions and Reagents, 55th Edition, GOEL Publishing House, 2017.
9. W. Carruthers, Some Modern Methods of Organic Synthesis, Cambridge University Press, 4th Edition, Reprint 2004.
10. Jonathan Clayden, Nick Greeves and Stuart Warren, Organic Chemistry, Oxford University Press, 2nd Edition, 2012.
11. Francis A. Carey and Richard J, Advanced Organic Chemistry, Part B - Sundberg, 4th Edition, Reprint 2001.
12. J. March, Advanced Organic Chemistry, Wiley Inter Science, 4th Edition, Reprint 2001.
13. R. K. Mackie and D. M. Smith, Guide book to Organic Synthesis, Longman Publication, Reprint 1990.
14. R. O. C. Norman, Principles of Organic Synthesis, Chapman and Hall, London, 2nd Edition, Reprint 1980.
15. E. S. Gould, Structure and Mechanism, Copyright, 1959.

OER:

1. Infowledge - https://www.youtube.com/watch?v=CdeBCfkSTJg (Crams rule - CSIR problems)
2. Infowledge - https://www.youtube.com/watch?v=3ATGcugIYCo (Prelogs rule – CSIR problems)
3. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5(P05-Reaction intermediates)
4. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P09-Named reactions)
5. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P014-Retrosynthesis)
6. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5(P01-Asymmetric synthesis)

SEMESTER III

PICHG20 - IEP - RESEARCH METHODOLOGY

Year: II **SEM:** III	**Course Code** PICHG20	**Title of the Course** Research Methodology	**Course Type** Theory	**Course Category** Independent Elective	**H/W** Own Pace	**Credits** 2	**Marks** 100

Learning Objectives:

- To introduce the purpose and importance of research.
- To gain information about the various sources of literature.
- To learn the scientific method of collecting data and to compute statistical parameters to arrive at meaningful conclusions.
- To emphasize the importance of ethics in research and chemical safety.

Course Outcomes:

The Learners will be able to

1. Define research and its objectives, illustrate hypothesis testing, and draw the research plan.
2. Carry out literature search offline and online to fix the research problem and illustrate the importance of IF, SCI, h index and i-index.
3. Apply statistical analysis in research methodology.
4. Describe the general format of thesis writing and the research ethics to be followed.

5. Illustrate the safety measures to be taken in handling toxic, inflammable and explosive chemicals.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I

1.1 Scope of research - research methodology - definition of research, purpose of research. (K1, K2 & K3)

1.2 Types of research - descriptive vs analytical, applied vs fundamental, quantitative vs qualitative, conceptual vs empirical and other types of research. (K1, K2 & K3)

1.3 Research design - planning of research, selection of a problem for research. (K1, K2, K3 & K4)

1.4 Research process - steps involved. (K1, K2 & K3)

1.5 Problems and hypothesis in research - identification of problems, sources, factors influencing selection of problems. (K1, K2, K3 & K4)

1.6 Development and testing of hypothesis. (K1, K2, K3 & K4)

Unit II

2.1 Literature search techniques - sources of information, need for reviewing literature. (K1, K2 & K3)

2.2 Primary, secondary and tertiary sources - journals, E-journals, journal access, journal abbreviations, chemical abstracts, Beilstein, reviews, monographs, dictionaries, text books. (K1, K2 & K3)

2.3 UGC infonet, E-resources. (K1, K2, K3 & K4)

2.4 Search engines - Google scholar, chemical industry, Wiki-databases, chemSpider, Science Direct, SciFinder, Scopus, SPN, Reaxys, orbit.com, Thompson innovations. (K1, K2, K3 & K4)

2.5 Indices - subject index, substance index, author index, formula index and other indices with examples, searches through structure, knowledge of national and international journals. (K1, K2, K3 & K4)

2.6 Impact Factor, Citation-Index, h Index, I-index, SCI Journals. (K1, K2, K3 & K4)

Unit III

3.1 Data Analysis - errors in chemical analysis, types of errors, precision and accuracy. (K1, K2, K3 & K4)

3.2 Significant figures, measures of central tendency - arithmetic mean, median, mode. (K1, K2, K3 & K4)

3.3 Methods of dispersion - standard deviation, co-efficient of variation (discrete series and continuous series). (K1, K2, K3 & K4)

3.4 Comparison of results - t- test, F- test and chi square test. (K1, K2, K3 & K4)

3.5 Correlation - coefficient of correlation, linear regression - coefficient of regression. (K1, K2, K3 & K4)

3.6 Multiple linear regression. (K1, K2, K3 & K4)

Unit IV

4.1 Writing a thesis: The general format - page and chapter format - the use of quotations - footnotes and figures - referencing - appendices - references. (K1, K2 & K3)

4.2 Research Ethics - academic honesty, intellectual ownership - copy right, royalty. (K1, K2 & K3)

4.3 Intellectual property rights and patent law. (K1, K2 & K3)

4.4 Plagiarism - responsibility, reproduction of published material and accountability of the researcher, situation that raises ethical issues, freedom and privacy from coercion. (K1, K2 & K3)

4.5 Ethics in relation to other people, role of research participant. (K1, K2 & K3)

4.6 Software for detecting plagiarism. (K1, K2 & K3)

Unit V

5.1 Concepts of chemical safety: Chemical safety and ethical handling of chemicals. (K1, K2, K3 & K4)

5.2 Safe working procedure and protective environment. (K1, K2, K3 & K4)

5.3 Emergency procedure and first aid, laboratory ventilation, safe storage and handling of hazardous chemical. (K1, K2, K3 & K4)

5.4 Procedure for working with substances that pose hazards, flammable or explosive hazards. (K1, K2, K3 & K4)

5.5 Procedures for working with gases at pressures above or below atmosphere. (K1, K2, K3 & K4)

5.6 Safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals. (K1, K2, K3 & K4)

Reference Books:

1. Anderson, Thesis and Assignment Writing, Wiley Eastern Ltd., 1st Edition, Eighth Reprint 1987.
2. C. R. Kothari, Research Methodology, Wiley Eastern Ltd., Fourth Reprint 1989.
3. R. P. Misra, Research Methodology, Concept Publishing Company, New Delhi, 2002.
4. R. Gopalan, Thesis Writing, Vijay Nicole Imprints Private Limited, 2005.
5. P. Ramadass and A. Wilson Aruni, Research and Writing: Across the Disciplines, MJP Publishers, 2009.

6. N. Gurumani, Scientific Thesis Writing and Paper Presentation, MJP Publishers, Chennai, 2010.
7. S. C. Gupta and V. K. Kapoor, Fundamentals of Mathematical Statistics, Sultan Chand & Sons, New Delhi, 1999.
8. G. W. Snedecor and W. G. Cochrans, Statistical Methods, Lowa State University Press, 1967.
9. R. Panneerselvam, Research Methodology, Prentice Hall of India Private Ltd., New Delhi, Abridged, 1st January 2013.
10. Satarkar, S. V., Intellectual Property Rights and Copyrights, Ess Ess Publications, 2003.
11. Anthony M Graziano and Michael L Rau, Research Methods: A Process of Inquiry, Prentice Hall, 2006.
12. P. Rajammal and P. Devadoss, A Hand Book of Methodology of Research, R. M. M. Vidya Press, 1976.
13. H. F. Ebel, C. Bliefert and W. E. Russey, The Art of Scientific Writing: From Students Reports to Professional Publications in Chemistry and Related Fields, VCH, Weinheim, New York, 1987.

OER:

1. https://www.google.com/url?sa=t&source=web&rct=j&url=https://dinus.ac.id/repository/docs/ajar/Kothari_-_Research_Methodology_Methods_and_Techniques_-_2004.pdf&ved=2ahUKEwiS3M7WsMzrAhWDcn0KHZU7AV8QFjAKegQICBAB&usg=AOvVaw00Lf_VgXYG-96PVmSGC0DG
2. http://www.insaindia.res.in/pdf/Ethics_Book.pdf - pages 35-43
3. http://ccc.chem.pitt.edu/wipf/Web/HCH.pdf

SEMESTER IV

PCCHM20 - NATURAL PRODUCTS AND BIOORGANIC CHEMISTRY

Year: II **SEM:** IV	**Course Code** PCCHM20	**Title of the Course** Natural Products and Bioorganic Chemistry	**Course Type** Theory	**Course Category** Core	**H/W** 5	**Credits** 4	**Marks** 100

Learning Objectives:

- To impart knowledge on amino acids, peptides and proteins.
- To study in detail the chemistry of nucleic acids and enzymes.

Course Outcomes:

The Learners will be able to

1. Examine the synthesis and reactions of selected heterocyclic pigments, nucleic acids, vitamins and alkaloids.
2. Evaluate the biosynthesis and metabolism of lipids, cholesterol and hormones.

3. Explain the metabolic pathway of amino acids and proteins and to analyze the structural aspects of proteins.
4. Elaborate the role and metabolism of nucleic acids, genetic code, transcription and translation.
5. Describe the structure and biological role of enzymes (α-chymotrypsin) and cofactors.

CO	PSO					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Synthesis and reactions of imidazole, oxazole, thiazole. (K1, K2, K3, K4, K5 & K6)
1.2 Pigments - synthesis and reactions of flavones, isoflavones, anthocyanins. (K1, K2, K3, K4, K5 & K6)
1.3 Nucleic acids - synthesis and reactions of pyrimidines (cytosine and uracil only) (K1, K2, K3, K4, K5 & K6)
1.4 Purines (adenine and guanine only). (K1, K2, K3, K4, K5 & K6)
1.5 Vitamins - synthesis of Vitamin A (Reformatsky and Wittig reaction methods only), synthesis of Vitamin B_1 - thiamine. (K1, K2, K3, K4, K5 & K6)
1.6 Alkaloids - total synthesis of morphine, quinine and papaverine. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Lipids - classification (K1, K2, K3, K4. & K5)
2.2 Chemical properties - saponification, rancidity, oxidation, hydrogenation, dehydration and halogenations reactions - iodine number, saponification number, acetyl number. (K1, K2, K3, K4 & K5)
2.3 Synthesis and degradation of neutral lipids - metabolism of lipids - beta oxidation of fatty acids. (K1, K2, K3, K4 & K5)
2.4 Biosynthesis of fatty acids. (K1, K2, K3, K4 & K5)

2.5 Metabolism of cholesterol, biosynthesis of cholesterol. (K1, K2, K3, K4 & K5)

2.6 Biosynthesis of steroid hormones - conversion of cholesterol to progesterone, oestrone and testosterone. (K1, K2, K3, K4, & K5)

Unit III **(15 Hours)**

3.1 Amino acids - metabolism of amino acids - oxidative deamination, transamination reactions and urea cycle. (K1, K2, K3, K4, K5 & K6)

3.2 Peptides - synthesis of tripeptide - solid phase peptide synthesis - Merrifield synthesis. (K1, K2, K3, K4, K5 & K6)

3.3 Separation and purification of proteins - dialysis, gel filtration and electrophoresis. (K1, K2, K3, K4, K5 & K6)

3.4 Structural aspects of proteins - determination of primary structure by end group analysis. (K1, K2, K3, K4, K5 & K6)

3.5 Determination of secondary and tertiary structure of proteins by XRD, cryoscopy method and NMR. (K1, K2, K3, K4, K5 & K6)

3.6 Biosynthesis of amino acids - phenylalanine, tyrosine and proline only. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Nucleic acids - introduction - types of nucleic acids - structure of nucleosides and nucleotides - DNA and RNA-polynucleotide chain - structural features of DNA and RNA - Watson-Crick Model. (K1, K2, K3, K4 & K5)

4.2 Chemical and enzymatic hydrolysis of nucleic acids - DNA sequence determination by chemical and enzymatic methods. (K1, K2, K3, K4 & K5)

4.3 DNA metabolism - replication - mechanism - mutation. (K1, K2, K3, K4 & K5)

4.4 Transcription - synthesis of RNA and its mechanism. (K1, K2, K3, K4 & K5)

4.5 Genetic code - origin and evolution, salient features - Wobble hypothesis. (K1, K2, K3, K4 & K5)

4.6 Biosynthesis of proteins (translation). (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Enzyme chemistry - enzyme mechanism of alpha chymotrypsin. (K1, K2, K3, K4, K5 & K6)

5.2 Immobilized enzyme technology - enzymes in synthetic organic chemistry. (K1, K2, K3, K4, K5 & K6)

5.3 Coenzyme chemistry - prosthetic groups, apo enzymes - structure, biological function and mechanism of reactions catalyzed by coenzyme A and thiamine pyrophosphate. (K1, K2, K3, K4, K5 & K6)

5.4 Structure, biological function and mechanism of reactions catalyzed by pyridoxal phosphate and NAD^+. (K1, K2, K3, K4, K5 & K6)

5.5 Structure, biological function and mechanism of reactions catalyzed by NADP and FAD. (K1, K2, K3, K4, K5 & K6)

5.6 Structure, biological function and mechanism of reactions catalyzed by lipoic acid and Vitamin B_{12} (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. I. L. Finar, Organic Chemistry, Vol. II, ELBS Publication, 5th Edition, 2005.
2. Raj K Bansal, Heterocyclic Chemistry, New Age International, 3rd Edition, Reprint 2005.

3. Nelson and Cox (Lehninger), Principles of Biochemistry, Freeman and Company, 4th Edition, 2005.
4. Robert K. Murray, Daryl K. Granner, Peter A. Mayes, Victor W. Rodwell, Harper's Illustrated Biochemistry, McGraw-Hill, 26th Edition, 2003.
5. Pamela C. Champe and Richard A. Harvey, Lippincott's Illustrated Reviews: Biochemistry, 3rd Edition, 2004.
6. U. Satyanarayana and U. Chakrapani, Fundamentals of Biochemistry, Books & Allied (P) Ltd., Reprint 2008.
7. Dr. R. Hannah Sulochana, Principles of Biochemistry, PBS Private Limited Chennai, 1st Edition, 2010.
8. A. C. Deb, Fundamentals of Biochemistry. New Central Book Agency (P) Ltd., 10th Edition, 2011.
9. Hermann Dugas, Bioorganic Chemistry - A Chemical Approach to Enzyme Action, Springer, 3rd Edition, Reprint 2007.
10. P. S. Kalsi and Sangeeta Jagtap, Pharmaceutical, Medicinal and Natural Product Chemistry, Narosa Publishing House, New Delhi, 2013.
11. Gurdeep R. Chatwal, Organic Chemistry of Natural Products (Vol. I & II), Himalaya Publishing House, Mumbai, 1st Edition, Reprint 2003.
12. R. C. Dubey and D. K. Maheshwari, A Textbook of Microbiology, S. Chand and Company Ltd., Revised Edition, 2010.

OER:

1. https://www.khanacademy.org/test-prep/mcat/biomolecules/enzyme-structure-and-function/v/an-introduction-to-enzymes-and-catalysis (Enzyme and Catalysis).
2. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=2 (Lipid metabolism).
3. https://bio.libretexts.org/Bookshelves/Biochemistry/Book%3A_Biochemistry_Free_and_Easy_(Ahern_and_Rajagopal)/06%3A_Metabolism_I__Oxidative%2F%2FReductive_Processes/6.13%3A_Metabolism_of_Fat (Metabolism of fat)
4. https://nptel.ac.in/courses/104/102/104102016/ (Structure and function of Biomolecules)
5. https://nptel.ac.in/courses/104/102/104102009/ (Structure of proteins)
6. https://nptel.ac.in/courses/104/103/104103121/ (Nucleic acids)

SEMESTER IV

PCCHN20 - SOLID STATE CHEMISTRY AND NUCLEAR CHEMISTRY

Year: II **SEM:** IV	**Course Code** PCCHN20	**Title of the Course** Solid State Chemistry and Nuclear Chemistry	**Course Type** Theory	**Course Category** Core	**H/W** 5	**Credits** 4	**Marks** 100

Learning Outcomes:

- To know about the structure and properties of solids.
- To gain knowledge on nuclear chemistry and nuclear reactors.

Course Outcomes:

The Learners will be able to

1. Sketch the structures of perovskite, CdI, NiAs, spinels, explain electrical, magnetic and optical properties of solids, compare different methods of solid-state reactions and demonstrate selected single crystal growth techniques.
2. Discuss the magnetic properties of nuclides.

3. Describe quark theory and salient features of nuclear models.
4. Illustrate the types of nuclear reactions, explain the applications of radioisotopes in neutron activation analysis, isotope dilution analysis and age determination.
5. Compare the different types of particle detectors, accelerators and explain the knowledge on Nuclear Waste Management.

CO	PSO					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	M	M	M	H	H
CO2	H	M	M	M	H	M
CO3	H	L	M	M	H	M
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	**2**	**3**	**4**	**5**	**6**
CO1	H	H	H	M	H	M
CO2	H	H	H	L	M	M
CO3	H	H	H	M	M	H
CO4	H	H	H	M	H	M
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Structure of solids - Miller planes, Miller indices for hexagonal systems, distance between planes. (K1, K2, K3, K4, K5 & K6)
1.2 Reciprocal lattice, XRD instrumentation, XRD - analysis of pattern. (K1, K2, K3, K4, K5 & K6)
1.3 Structure of perovskite, cadmium iodide, nickel arsenide, spinels and inverse spinels. (K1, K2, K3, K4, K5 & K6)
1.4 Diffusion, diffusion co-efficient, diffusion mechanisms - vacancy and interstitial diffusion. (K1, K2, K3, K4, K5 & K6)
1.5 Growing single crystals - crystal growth from solution, growth from melt and chemical vapour deposition technique. (K1, K2, K3, K4, K5 & K6)
1.6 Electronic properties of solids - Hall Effect and its applications, pyroelectricity, piezo electricity and ferro electricity. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Magnetic properties of solids - hysteresis loss and loops. (K1, K2, K3, K4 & K5)
2.2 Types of magnetic behavior - dia, para, ferro, anti-ferro, ferri magnetism - ferrites, garnets. (K1, K2, K3, K4 & K5)

2.3 Optical properties of solids - luminescence and phosphors. (K1, K2, K3, K4 & K5)

2.4 Lasers - ruby laser, neodymium laser. (K1, K2, K3, K4 & K5)

2.5 Solid state electrolyte - β-alumina - application of solid state electrolytes. (K1, K2, K3, K4 & K5)

2.6 Solid-state reactions - formation of spinel ($MgAl_2O_4$), co-precipitation and sol-gel method ($LiNbO_3$, silica). (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 The quark theory - quarks - classification, mass and charge, quark-quark gluon interaction. (K1, K2, K3, K4, K5 & K6)

3.2 The magnetic properties of the nucleus - Bohr magneton, nuclear magneton, the neutron magnetic moment and the structure of the nucleon. (K1, K2, K3, K4, K5 & K6)

3.3 The net magnetic moments of the nuclei - the spin I, the magnetic moment μ_I and Nordheim rules. (K1, K2, K3, K4, K5 & K6)

3.4 Salient feature of the liquid drop model with derivations. (K1, K2, K3, K4, K5 & K6)

3.5 Fermi - gas model, collective model. (K1, K2, K3, K4, K5 & K6)

3.6 Nuclear reaction - cross-section, Q value, threshold energy and compound nucleus theory. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Bethe's notation, types of nuclear reactions - direct reactions, photonuclear and thermo nuclear reactions. (K1, K2, K3, K4 & K5)

4.2 Modes of radioactive decay, nuclear isomerism and isomeric transition, internal conversion. (K1, K2, K3, K4 & K5)

4.3 Stellar energy, the nucleosynthesis of light and heavy elements, hydrogen burning, carbon burning, the e, s, r, p and x processes. (K1, K2, K3, K4 & K5)

4.4 Separation of isotopes - boron isotope - isotope exchange and laser irradiation. (K1, K2, K3, K4 & K5)

4.5 Separation of uranium isotopes - ultracentrifugation and laser irradiation. (K1, K2, K3, K4 & K5)

4.6 Analytical applications of radioisotopes as traces - isotope dilution analysis and neutron activation analysis, age determination by tritium and carbon-14 content. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Hot atom chemistry and chemical effect of radioactive decay. (K1, K2, K3, K4, K5 & K6)

5.2 Detectors: Cloud chamber, bubble chamber, Geiger-Muller counter, scintillation and Cherenkov counters. (K1, K2, K3, K4, K5 & K6)

5.3 Particle accelerators - linear accelerators, cyclotron and synchrotron. (K1, K2, K3, K4, K5 & K6)

5.4 India's three stage nuclear power programme - pressurized heavy water reactor, fast breeder reactor, and thorium-based reactor. (K1, K2, K3, K4, K5 & K6)

5.5 Reprocessing of spent fuels: Recovery of uranium and plutonium. (K1, K2, K3, K4, K5 & K6)

5.6 Nuclear waste management - low level, intermediate level, high level wastes and ultimate disposal. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. A. R. West, Solid State Chemistry and its Application, John Wiley, Reprint 2011.
2. Smart & Moore, An Introduction to Solid State Chemistry, Chapman & Hall, 4th Edition, Reprint 2012.
3. D. K. Chakrabarty, Solid State Chemistry, New Age International, Reprint 2017.
4. Glen E. Rodgers, Inorganic and Solid State, Brooks/Cole Cengage Learning Publication, Indian Reprint 2011.
5. U. N. Dash, Nuclear Chemistry, Sultan Chand and Son Publication, First Edition, 1991.
6. H. J. Arnikar, Essentials of Nuclear Chemistry, New Age International, Reprint 2011.
7. R. K. Dave, Nuclear Chemistry, Campus Book International, 2006.
8. Maheshwar Sharon, Madhuri Sharon, Nuclear Chemistry, Anne Books Pvt. Ltd., 2nd Edition, Reprint 2018.
9. Walter D Loveland, Modern Nuclear Chemistry, Wiley, Reprint 2017.

OER:

1. http://wwwchem.uwimona.edu.jm/courses/binsalts.html
2. http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html
3. http://www.barc.gov.in/about/anushakti_sne.html
4. https://www.khanacademy.org/science/cosmology-and-astronomy/stellar-life-topic/stellar-life-death-tutorial/v/lifecycle-of-massive-stars

SEMESTER IV

PCCHO20 - THERMODYNAMICS

Year: II **SEM:** IV	**Course Code** PCCHO20	**Title of the Course** Thermodynamics	**Course Type** Theory	**Course Category** Core	**H/W** 5	**Credits** 5	**Marks** 100

Learning Objectives:

- To give an in-depth knowledge on thermodynamics.
- To understand the concepts of statistical thermodynamics.
- To give insight into the applications of the M-B, B-E and F-D statistics.

Course Outcomes:

The Learners will be able to

1. Determine the partial molar properties, activity and activity coefficient of non-electrolytes, and standard free energies.
2. Illustrate the relationship between microscopic properties of individual atoms and molecules with macroscopic thermodynamic observables and derive the different types of distribution laws.

3. Derive different forms of molecular partition function, heat capacity of solids and explain law of equipartition of energy.
4. Distinguish the nuclear spin states of hydrogen and deuterium, explain electron gas in metals and blackbody radiation, and apply spectroscopic data for statistical thermodynamics.
5. Explain the concept of non-equilibrium thermodynamics, and derive entropy production in chemical reactions and open systems.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Partial molar properties - partial molar free energy - partial molar volume and partial molar heat content - their significance and determination of these quantities - determination of partial molar properties. (K1, K2, K3, K4, K5 & K6)

1.2 Chemical potential - variation of chemical potential with temperature and pressure, Duhem Margules equation. (K1, K2, K3, K4, K5 & K6)

1.3 Free energy - standard free energy - determination of standard free energies from entropy values, equilibrium constant and ionization method. (K1, K2, K3, K4, K5 & K6)

1.4 Fugacity and activity - definition of fugacity, variation of fugacity with temperature and pressure. (K1, K2, K3, K4, K5 & K6)

1.5 Concept of activity and activity co-efficient - choice of standard states. (K1, K2, K3, K4, K5 & K6)

1.6 Determination of activity and activity co-efficient of non-electrolytes by Henry's distribution law and vapor pressure measurements. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Thermodynamic and mathematical probability - Sterling approximation -Lagrange's method of indeterminate multipliers. (K1, K2, K3, K4 & K5)

2.2 Distribution and most probable distributions - distinguishable and indistinguishable particles. (K1, K2, K3, K4 & K5)

2.3 Statistical mechanics - Maxwell-Boltzmann Distribution - derivation and applications (K1, K2, K3, K4 & K5)

2.4 Bose-Einstein and Fermi Dirac distribution laws - derivations and applications - comparison of the distribution laws. (K1, K2, K3, K4 & K5)

2.5 Relation between partition and thermodynamic functions. (K1, K2, K3, K4 & K5)

2.6 Different types of ensembles and ensemble averaging. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Partition function - factorization of molecular partition function, partition functions for mixture of gases. (K1, K2, K3, K4, K5 & K6)

3.2 Evaluation of the independent molecular partition function - translational, rotational, vibrational partition function. (K1, K2, K3, K4, K5 & K6)

3.3 Evaluation of electronic and nuclear partition function. (K1, K2, K3, K4, K5 & K6)

3.4 Law of equipartition of energies. (K1, K2, K3, K4, K5 & K6)

3.5 Heat capacity of solids - specific heat capacity of solids. (K1, K2, K3, K4, K5 & K6)

3.6 Determination of heat capacity of solids at low temperature - Einstein model and Debye model. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Nuclear spin statistics - ortho-para nuclear states. (K1, K2, K3, K4 & K5)

4.2 Ortho-para hydrogen, nuclear spin statistics of deuterium. (K1, K2, K3, K4 & K5)

4.3 Investigation on system containing indistinguishable particles - electron in metals. (K1, K2, K3, K4 & K5)

4.4 Black body radiation - Planck's distribution law, Stefan-Boltzmann law, Wein's law. (K1, K2, K3, K4 & K5)

4.5 Application of statistical thermodynamics. (K1, K2, K3, K4 & K5)

4.6 Uses of spectroscopic and structural data to calculate thermodynamic functions. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Non equilibrium thermodynamics: Irreversible thermodynamics - postulates of non-equilibrium thermodynamics. (K1, K2, K3, K4, K5 & K6)

5.2 Conservation of mass and energy. (K1, K2, K3, K4, K5 & K6)

5.3 Entropy production - entropy production in chemical reactions - entropy flow in open systems. (K1, K2, K3, K4, K5 & K6)

5.4 Flux and Force - transformation properties of rates and affinities. (K1, K2, K3, K4, K5 & K6)

5.5 Linear laws relative to fluxes and forces - Onsager's reciprocity relation(K1, K2, K3, K4, K5 & K6)

5.6 Curie's theorem, relaxation phenomenon. (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. Terrell L. Hill, An Introduction to statistical Thermodynamics, Dover Publications, First South Asian Edition, 2008.
2. B. G. Kyle, Chemical and Process Thermodynamics, Prentice Hall of India, 3rd Edition, 2004.
3. Samuel Glasstone, Thermodynamics for Chemists, East-West Press, Reprint 2017.

4. M. C. Gupta, Statistical Thermodynamics, New Age International, 2nd Edition, 2003.
5. R. C. Srivatsava, Subit K. Saha, Abhay K. Jain, Thermodynamics: A Core Course, PHC Pvt. Ltd., 2nd Edition, 2005.
6. J. Rajaram, J. C. Kuriacose, Chemical Thermodynamics, Dorling Kindersley Pvt. Ltd., Pearson Education Publisher, 2013.
7. Evelyn Guha, Basic Thermodynamics, Narosa Publishing House, 1st Edition, 2000.
8. P. C. Rakshit, Thermodynamics, The New Book Stall, 4th Edition, 1983.
9. Y. V. C Rao, An Introduction to Thermodynamics, New Age International Pvt. Ltd., 1st Edition, 1993.
10. Sears Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Narosa Publishing House, 3rd Edition, 1975.
11. R. P. Rastogi and R. R. Misra, An Introduction to Chemical Thermodynamics, Vikas Publishing House Pvt. Ltd., 1995, Reprint 2007.
12. Raza, Tahir-Kheli, General and Statistical thermodynamics, e-ISBN - 978-3-642-21481-3, Springer 2012.

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1. https://ethz.ch/content/dam/ethz/special-interest/chab/physical-chemistry/epr-dam/documents/education/statistical-thermodynamics/stat_TD.pdf.
2. http://ursula.chem.yale.edu/~batista/classes/vaa/vaa.pdf (Statistical methods and thermodynamics)
3. https://physics.info/planck/ (Black body radiation)
4. https://www.intechopen.com/books/non-equilibrium-particle-dynamics/fundamentals-of-irreversible-thermodynamics-for-coupled-transport.
5. https://arxiv.org/pdf/1906.07656.pdf (Spin statistics)

SEMESTER IV

PECHG20 - ELECTIVE IV A: ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

Year: II **SEM:** IV	**Course Code** PECHG20	**Title of the Course** Organometallic and Bioinorganic Chemistry	**Course Type** Theory	**Course Category** Core Elective	**H/W** 5	**Credits** 4	**Marks** 100

Learning Objectives:

- To expose the students to the principles and reactions involved in Organometallic chemistry.
- To understand the role of catalysts in different types of reactions.
- To have a clear understanding on bioinorganic compounds.

Course Outcomes:

The Learners will be able to

1. Explain the preparation, properties, structure and bonding of organometallic complexes and appraise 18 electron rule and EAN rule for metal carbonyls.
2. Explain the mechanism of organometallic reactions, rearrangement reactions of aluminium and tin compounds.
3. Appraise the role of transition metal catalysts in industrial processes.
4. Evaluate the role of oxygen transport, ion transport and electrolytic balance in organisms, and review nitrogen fixation.
5. Elaborate on the biological role of metalloenzymes, and the importance of metals used for diagnosis and treatment of cancer.

CO	PSO					
	1	2	3	4	5	6
CO1	H	M	L	H	H	H
CO2	H	M	L	H	H	H
CO3	H	M	L	H	H	H
CO4	H	M	L	H	H	H
CO5	H	M	L	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Introduction - 18 electron rule and EAN rule - calculation, hapacity - definition. (K1, K2, K3, K4, K5 & K6)

1.2 Metal carbonyl complexes and poly nuclear carbonyl complexes - preparation, properties, structure and bonding. (K1, K2, K3, K4, K5 & K6)

1.3 Carbonylate ion, carbonyl hydride complex – preparation, properties, structure and bonding. (K1, K2, K3, K4, K5 & K6)

1.4 Nitrosyl complex, metal alkyls - preparation and properties, structure and bonding. (K1, K2, K3, K4, K5 & K6)

1.5 Carbenes, carbynes and carbides, non-aromatic alkenes and alkyne complexes - preparation and properties. (K1, K2, K3, K4, K5 & K6)

1.6 Metallocenes - preparation and properties, structure and bonding. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Addition reactions - 1,2 addition to double bonds. (K1, K2, K3, K4 & K5)

2.2 Carbonylation and decarbonylation. (K1, K2, K3, K4 & K5)

2.3 Oxidative addition reactions, reductive elimination reactions. (K1, K2, K3, K4 & K5)

2.4 Substitution reactions of octahedral complexes and their mechanisms. (K1, K2, K3, K4 & K5)

2.5 Insertion reaction, rearrangement reactions of aluminium and tin compounds and their mechanisms. (K1, K2, K3, K4 & K5)

2.6 Fluxional isomerism - definition, examples and mechanism. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Hydrogenation of olefins (Wilkinson's catalyst), modification of the original catalyst. (K1, K2, K3, K4, K5 & K6)

3.2 Hydroformylation of olefins using cobalt and rhodium catalyst (oxo process). (K1, K2, K3, K4, K5 & K6)

3.3 Oxidation of olefins to aldehydes and ketones (Wacker process). (K1, K2, K3, K4, K5 & K6)

3.4 Cyclo oligomerisation of acetylene using Nickel catalyst (Reppe's catalyst) (K1, K2, K3, K4, K5 & K6)

3.5 Olefin isomerization and its mechanism. (K1, K2, K3, K4, K5 & K6)

3.6 Olefin metathesis and polymer bound catalyst. (K1, K2, K3, K4, K5 K6)

Unit IV **(15 Hours)**

4.1 Metallo porphyrin and respiration (cytochromes). (K1, K2, K3, K4 & K5)

4.2 Interaction between heme and dioxygen, structure and function of haemoglobin. (K1, K2, K3, K4 & K5)

4.3 Ferredoxin and rubredoxin, blue copper proteins - structure and function. (K1, K2, K3, K4 & K5)

4.4 Ion transport in membranes, Na-K balance. (K1, K2, K3, K4 & K5)

4.5 Calcium in living cells (transport and regulation), selectivity of Ca^{2+} over Mg^{2+}.(K1, K2, K3, K4 & K5)

4.6 Nitrogen fixation - atmospheric, industrial and biological. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Biological role of metalloenzymes - carboxy peptidases. (K1, K2, K3, K4, K5 & K6)

5.2 Biological role of carbonic anhydrase. (K1, K2, K3, K4, K5 & K6)

5.3 Biological importance of catalase. (K1, K2, K3, K4, K5 & K6)

5.4 Biological role of peroxidase. (K1, K2, K3, K4, K5 &K6)

5.5 Oxotransferase enzymes - xanthine oxidase - biological role. (K1, K2, K3, K4, K5 & K6)

5.6 Metals used for diagnosis and chemotherapy with particularreference to anticancer drugs (platinum ammine halides, metallocenes and their halides). (K1, K2, K3, K4, K5 & K6)

Reference Books:

1. R. Gopalan, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., Reprint 2008.
2. Asim K. Das, Bioinorganic Chemistry, Books and Allied Pvt. Ltd., Kolkota, Reprint 2013.
3. Gary Miessler, Paul J. Fischer, Donald A. Tarr, Inorganic Chemistry, Pearson, 5th Edition, 2014
4. B. E. Douglas DH McDaniel's and Alexander, Concepts and Models of Inorganic Chemistry, Wiley Publication, 2nd Edition, Reprint 2006.

5. Ivano Bertini, Harry B Gray, Stephen J Lippard, Joan Selverstone Valentine, Bioinorganic Chemistry, University Science Books, Mill Valley, California, 1st Edition, 1994
6. M. C. Shrivers, P. W. Atkins, C. H. Langford, Inorganic Chemistry, Oxford University Press, 3rd Edition, Reprint 2002.
7. J. Huheey, Inorganic Chemistry, Pearson, 4th Edition, 2006.
8. Wahid U. Malik, G. D. Tuli, R. D. Madan, Selected Topics in Inorganic Chemistry, S. Chand and Co., New Delhi, Reprint 1993.
9. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley and Sons, 5th Edition, 1988.
10. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, W. B. Saunders Co., 1977.
11. S. F. A. Kettle, Coordination Chemistry, ELBS, Reprint 1975.
12. F. Basolo and RG Pearson, Mechanism of Inorganic Reactions, Wiley, 1967.

OER:

1. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-03-Mechanism of substitution reactions)
2. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-15-Iron transport, nitrogen fixation)
3. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5 (P-11-Carbonyls and nitrosyls)
4. file:///E:/E%20books/Inorganic_Chemistry__Miessler___Tarr.pdf

SEMESTER IV

PECHH20 - ELECTIVE IVB: ORGANIC FARMING AND SOLID WASTE MANAGEMENT

Year: II **SEM:** IV	**Course Code** PECHH20	**Title of the Course** Organic Farming and Solid Waste Management	**Course Type** Theory	**Course Category** Core Elective	**H/W** 5	**Credits** 4	**Marks** 100

Learning Objectives:

- To understand the importance of solid waste management.
- To learn about hazardous waste management.
- To get a thorough knowledge on the concept of organic farming, components and practices.

Course Outcomes:

The Learners will be able to

1. Elaborate the concept of organic farming.
2. Explain the vision and importance of organic farming movements, apply vermicomposting process and prepare bio-fertilizers.

3. Evaluate the technology to approach the benefits of organic farming.
4. Explain the various aspects of solid waste management.
5. Demonstrate the methods to reduce hazards.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I **(15 Hours)**

1.1 Organic farming - concepts, relevance of organic farming to Indian agriculture. (K1, K2, K3, K4, K5 & K6)
1.2 Effects of green revolution, adverse effects of continuous use of chemicals. (K1, K2, K3, K4, K5 & K6)
1.3 Categories of organic farming, organic vs natural farming. (K1, K2, K3, K4, K5 & K6)
1.4 Essential characteristics of organic farming. (K1, K2, K3, K4, K5 & K6)
1.5 Key principles in organic farming system - components of organic farming systems. (K1, K2, K3, K4, K5 & K6)
1.6 Management of organic farming - research needs. (K1, K2, K3, K4, K5 & K6)

Unit II **(15 Hours)**

2.1 Principles and practices of organic farming. (K1, K2, K3, K4 & K5)
2.2 The vision and importance of organic farming movements. (K1, K2, K3, K4 & K5)
2.3 Guidelines for organic production system - organic farming practices - bulky organic manures. (K1, K2, K3, K4 & K5)
2.4 Role of micro-organisms (bio-fertilizers) in organic farming. (K1, K2, K3, K4 & K5)
2.5 Vermitechnology. (K1, K2, K3, K4 & K5)
2.6 Research advances in organic farming. (K1, K2, K3, K4 & K5)

Unit III **(15 Hours)**

3.1 Benefits of organic farming**.** (K1, K2, K3, K4, K5 & K6)
3.2 Nutritional values of organic foods. (K1, K2, K3, K4, K5 & K6)
3.3 Health benefits of organic foods. (K1, K2, K3, K4, K5 & K6)
3.4 SREP approach for promoting organic farming. (K1, K2, K3, K4, K5 & K6)
3.5 Use of organic practices in enhancing crop productivity. (K1, K2, K3, K4, K5 & K6)
3.6 Participatory technology development in organic farming. (K1, K2, K3, K4, K5 & K6)

Unit IV **(15 Hours)**

4.1 Solid Waste Management - introduction. (K1, K2, K3, K4 & K5)
4.2 Classification of solid wastes. (K1, K2, K3, K4 & K5)
4.3 Mismanagement and side effects. (K1, K2, K3, K4 & K5)
4.4 Physical and chemical characteristics. (K1, K2, K3, K4 & K5)
4.5 Waste collection, storage and transport. (K1, K2, K3, K4 & K5)
4.6 Waste disposal - types - composting, incineration, bio gasification. (K1, K2, K3, K4 & K5)

Unit V **(15 Hours)**

5.1 Plastics, bio medical and hazardous waste management. (K1, K2, K3, K4, K5 & K6)
5.2 Various types of plastics - plastic recycling and the environment. (K1, K2, K3, K4, K5 & K6)
5.3 Guidelines for the plastic waste hazards control. (K1, K2, K3, K4, K5 & K6)
5.4 Sources of biomedical waste - pathological waste, pharmaceutical wastes, genotoxic wastes, chemical wastes, radioactive wastes. (K1, K2, K3, K4, K5 & K6)
5.5 Measures to reduce hazards. (K1, K2, K3, K4, K5 & K6)
5.6 Household hazardous waste management - precautions, disposal, waste minimization. (K1, K2, K3, K4, K5 & K6)

References Books:

1. L. V. Hirevenkanagoudar, Extension Strategies for Promotion of Organic Farming, Agrotech Publishing Academy, 2007.
2. B. B. Hosetti, Prospects and Perspectives of Solid Waste Management, New Age International Publishers, 2006.
3. A. Kamala, D. L. Kanth Rao, Environmental Engineering, Water Supply, Sanitary Engineering and Pollution, Tata McGraw-Hill Publishing Ltd., New Delhi, 13th Reprint, 2002.
4. S. S. Dara, A Textbook of Environmental Chemistry and Pollution Control, S. Chand & Company Ltd., 7th Edition, 2004.
5. B. K. Sharma, Environmental Chemistry, Goel Publishing House, Meerut, 2005.

OER:

1. http://agritech.tnau.ac.in/org_farm/orgfarm_introduction.html
2. https://www.nationalgeographic.com/environment/future-of-food/organic-farming-crops-consumers/
3. https://www.britannica.com/topic/organic-farming
4. https://www.conserve-energy-future.com/sources-effects-methods-of-solid-waste-management.php

5. https://ec.europa.eu/echo/files/evaluation/watsan2005/annex_files/WEDC/es/ES07CD.pdf
6. https://www.geo.lu.lv/fileadmin/user_upload/lu_portal/projekti/gzzf/videunilgtspejigaattistiba/VidZ1000/16.LECTURE-Solid_waste_management.pdf
7. http://www.indiaenvironmentportal.org.in/files/file/municipal%20solid%20waste%20management.pdf

SEMESTER IV

PCCHP20 - PRACTICAL IV: ORGANIC CHEMISTRY - II

Year: II **SEM:** IV	**Course Code** PCCHP20	**Title of the Course** Practical IV: Organic Chemistry – II	**Course Type** Practical	**Course Category** Core	**H/W** 3	**Credits** 3	**Marks** 100

Course Outcomes:

The Learners will be able to

1. Develop skills to perform two stage preparations of organic compounds and crystallize them.
2. Calculate the saponification value of oil.
3. Estimate the amount of the given organic compound.
4. Demonstrate simple chromatographic techniques.
5. Interpret the structure of organic compounds by analyzing spectral data.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Estimations:

1. Estimation of aniline
2. Estimation of phenol
3. Estimation of ethyl methyl ketone
4. Estimation of glucose (Bertrand's method)
5. *Estimation of amide
6. Estimation of glycine
7. Saponification value of an oil

Preparations:

1. Benzanilide from benzophenone
2. m-nitrobenzoic acid from methyl benzoate
3. m-nitrobenzoic acid from benzaldehyde
4. 2,4-dinitrophenylhydrazine from chlorobenzene
5. Acetyl salicylic acid from methyl salicylate
6. Benzilic acid from benzoin

*** Chromatographic Separations:**

1. Column chromatography- separation of dyes
2. Paper chromatography - separation of mixture of amino acids
3. Thin layer chromatography - separation of mixture of amino acids

Interpretation of spectra of 10 organic compounds

*** Not to be given for examination**

Reference Books:

1. Mann and Saunders, Laboratory Manual of Organic Chemistry, Pearson Education, 4th Edition, 2009.
2. Vogel's Textbook of Practical Organic Chemistry, Pearson Education, 5th Edition, 2003.
3. Raj K. Bansal, Laboratory Manual of Organic Chemistry, New Age International Publishers, 5th Edition, 2009.
4. Gnanaprakasam, Ramamurthy, Organic Chemistry Manual, Viswanathan S. Printers and Publishers Pvt. Ltd., New Edition, 2009.

OER:

1. https://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi
2. http://www.chemspider.com/
3. https://cssp.chemspider.com
4. https://www.khanacademy.org/science/class-11-chemistry-india/xfbb6cb8fc2bd00c8:in-in-organic-chemistry-some-basic-principles-and-techniques/xfbb6cb8fc2bd00c8:in-in-methods-of-purification-of-organic-compounds/v/calculating-retention-factors-for-tlc

Continuous Assessment - 40 marks

I C.A. - 50 Marks
II C.A. - 50 Marks
Average - 25 Marks
Performance during regular practicals - 10 Marks
Regularity in submission of observation note-book and Record - 5 Marks

CA Practical Examination - 50 Marks

Spectra - 5 Marks

Record - 5 Marks

Viva - 5 Marks

Estimation - 15 Mark

Preparation - 20 Marks

(Stage1 - Quantity (5 Marks), Quality (5 Marks), Stage2 - Quantity (4 Marks), Quality (4 Marks), Recrystallization - 2Marks)

Semester Practical Examination - 60 Marks

Spectra - 5 Marks
Record - 5 Marks
Viva - 5 Marks
Preparation - 20 Marks
Estimation - 25 Marks

Quantitative Estimation

Upto 2% - 25 Marks
2 - 3% - 20 Marks

3- 4% - 15 Marks
> 4% - 10 Marks

SEMESTER IV

PCCHQ20 - PRACTICAL V: INORGANIC CHEMISTRY - II

Year: II **SEM:** IV	**Course Code** PCCHQ20	**Title of the Course** Practical V: Inorganic Chemistry - II	**Course Type** Practical	**Course Category** Core	**H/W** 4	**Credits** 3	**Marks** 100

Course Outcomes

The Learners will be able to

1. Estimate the amount of metal ions in inorganic mixtures by volumetric and gravimetric methods.
2. Estimate the percentage of metals in ores and alloys by volumetric and gravimetric methods.
3. Prepare selected inorganic complexes.
4. Interpret the spectra of selected inorganic compounds.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Estimations:

1. Estimation of copper and nickel
2. Estimation of copper and zinc
3. Estimation of iron and nickel
4. Estimation of iron and magnesium
5. Estimation of iron and zinc

Preparations:

1. Hexaamminenickel(II) chloride
2. Bis(acetylacetonato)copper(II)
3. Hexaamminecobalt(III) chloride
4. Pentamminechlorocobalt(III) chloride
5. Tris(thiourea)copper(I) sulphate
6. Potassium tetrachlorocuprate(II)
7. *Potassium tris(oxalato)aluminate(III) trihydrate

***Analysis of alloys:**

1. Determination of percentage of copper and zinc in brass
2. Determination of percentage of chromium and nickel in stainless steel

***Analysis of ores:**

1. Determination of percentage of calcium and magnesium in dolomite
2. Determination of percentage of MnO_2 in pyrolusite

Interpretation of spectra of 10 inorganic compounds

*** Not to be given for examination**

Reference Books:

1. V. Venkateswaran, R. Veeraswamy, A.R. Kulandaivelu, Basic Principles of Practical Chemistry, Sultan Chand & Sons, Educational Publishers, 2012.
2. G. Svehla, B. Sivasankar, Vogel's Qualitative Inorganic Analysis, Pearson Publication, 7th Edition, 2012.
3. R. Mukhopadhyay and P. Chatterjee, Advanced Practical Chemistry, Arunabha Sen Books and Allied (P) Ltd., Kolkatta, Third Edition, 2007.

OER:

1. https://www.khanacademy.org/science/chemistry/chemical-reactions-stoichiome/limiting-reagent-stoichiometry/a/gravimetric-analysis-and-precipitation-gravimetry. (Gravimetric Analysis)
2. https://chem.libretexts.org/Courses/Northeastern_University/08%3A_Gravimetric_Methods/8.2%3A_Precipitation_Gravimetry. (Precipitation Gravimetry).
3. http://vlab.amrita.edu/?sub=2&brch=193&sim=348&cnt=1 (Estimation of Nickel).

Continuous Assessment - 40 Marks
I C.A. - 50 Marks
II C.A. - 50 Marks
Average - 25 Marks
Performance during regular practical - 10 Marks
Regularity in submission of observation note-book and Record - 5 Marks

CA Practical Examination - 50 Marks
Spectra -5 Marks
Record -5 Marks
Viva -5 Marks
Preparation -10 Marks (Quantity – 5 Marks, Quality – 5 Marks)
Quantitative Estimation - 25 Marks (Volumetric - 10 Marks & Gravimetric - 15 Marks)

Semester Practical Examination - 60 Marks
Spectra - 5 Marks
Record - 5 Marks
Viva-Voce - 5 Marks
Preparation - 20 Marks (Quantity - 10 Marks, Quality - 10 Marks)
Quantitative Estimation - 25 Marks (Volumetric - 10 Marks & Gravimetric - 15 Marks)

Gravimetric Estimation		**Volumetric Estimation**	
up to 2%	- 15 Marks	up to 1%	- 10 Marks
2 - 3%	- 13 Marks	1% to 2%	- 8 Marks
3- 4%	- 10 Marks	2% to 3%	- 5 Marks
> 4%	- 7 Marks	>3%	- 4 Marks

SEMESTER IV

PCCHR20 - PRACTICAL VI: PHYSICAL CHEMISTRY - II

Year: II **SEM:** IV	**Course Code** PCCHR20	**Title of the Course** Practical VI: Physical Chemistry - II	**Course Type** Practical	**Course Category** Core	**H/W** 3	**Credits** 3	**Marks** 100

Course Outcomes:

The Learners will be able to

1. Apply laboratory skills to perform physico-chemical experiments.
2. Demonstrate acid-base, redox and precipitation titrations using conductometry and potentiometry.
3. Determine the pH of buffer solution potentiometrically and verify Ostwald dilution law and Onsager's equation.
4. Interpret the experimental results obtained by conductometric and potentiometric titrations.

5. Describe spectral methods to calculate force constant and interpret UV, IR and NMR spectra.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Experiments:

1. Determination of the strength of given weak acid by titrating potentiometrically with a strong base and determine dissociation constant of the weak acid to 1/4, 1/2 and 3/4 neutralization.
2. Determination of the strength of weak acid by titrating conductometrically against a standard sodium hydroxide solution.
3. Determination of pH values of the given buffer solutions by potentiometric method. You are provided with a buffer of known pH.
4. Determination of the strength of potassium iodide by titrating against standard potassium permanganate potentiometrically.
5. Verify the Onsager equation using the given solution and determine the equivalent conductance at infinite dilution.
6. Determination of the strength of ferrous ammonium sulphate solution by titrating against standard potassium permanganate potentiometrically.
7. Verify the Ostwald's dilution law and determine the dissociation constant of given acid.
8. Determination of the strength of potassium chloride by precipitation titration potentiometrically.

9. Titrate conductometrically the given mixture of strong and weak acids against a standard sodium hydroxide solution and determine the individual strength of the two acids in the mixture.
10. Determination of the strength of given strong acid by titrating potentiometrically with a strong base.
11. Determination of the strength of mixture of halides (KCl & KI) by precipitation titration potentiometrically.
12. Determination of the strength of given strong acid by titrating conductometrically with a strong base.
13. *****Titrate conductometrically the given mixture of HCl, CH_3COOH and $CuSO_4$. $5H_2O$ against NaOH and determine the individual strengths of the mixture.

***** Not to be given for examination.

Interpretation of spectra:

- Interpretation of UV-Visible spectra of simple molecules for the calculation of molecular data and identification of functional groups (5 typical spectra will be provided).
- IR and NMR spectral calculations of force constant - identification and interpretation of spectra (5 each in IR and NMR will be provided).

Reference Books:

1. V. Venkateswaran, R. Veeraswamy, A. R. Kulandaivelu, Basic Principles of Practical Physical Chemistry, Sultan Chand and Sons Educational Publishers, Reprint 2012.
2. V. K. Ahluwalia, Sunita Dhingra Adarsh Gulati, College Practical Chemistry, University Press (India) Private Limited, Reprint 2008.
3. B. Viswanathan, P. S. Raghavan, Practical Physical Chemistry, Viva Publishers, 2014.
4. J. B. Yadav, Advanced Practical Physical Chemistry, Krishna Prakashan Media (P) Ltd, 2015.

OER:

1. https://docs.google.com/presentation/d/1tc5iAxF-Kjt_P_lXeyFCQl2m-UHnY_t6CcLmdRBX1Ug/edit?usp=sharing
2. https://chem.pg.edu.pl/documents/175260/14212622/chf_epm_lab_1.pdf
3. http://web.iyte.edu.tr/~serifeyalcin/lectures/chem306/cn_3.pdf

Continuous Assessment - 40 Marks

I C.A. - 50 Marks

II C.A. - 50 Marks

Average - 25 Marks

Performance during regular practicals - 10 Marks

Regularity in submission of observation notebook and Record - 5 Marks

CA Practical Examination - 50 Marks

Spectra - 5 Marks

Conductometry - 17.5Marks

Potentiometry - 17.5 Marks

Record - 5 Marks

Viva-Voce - 5 Marks

Conductometry / Potentiometry (17.5 Marks)

Tabulation, Calculation, Graph - 7.5 Marks

Result - 10 Marks

Semester Practical Examination - 60 Marks

Spectra - 5 Marks

Conductometry - 20 Marks

Potentiometry - 20 Marks

Record - 10 Marks

Viva–Voce - 5 Marks

Conductometry / Potentiometry (20 Marks)

Tabulation, Calculation, Graph - 10 Marks

Result - 10 Marks

Error:

Upto 2% - 10 Marks

2% to 4% - 8 Marks

4% to 6% - 6 Marks

>6% - 5 Marks

SEMESTER IV

PICHH20 - IEP - CSIR-NET PREPARATORY COURSE IN PHYSICAL CHEMISTRY

Year: II **SEM:** IV	**Course Code** PICHH20	**Title of the Course** CSIR-NET Preparatory Course in Physical Chemistry	**Course Type** Theory	**Course Category** Independent Elective	**H/W** Own Pace	**Credits** 2	**Marks** 100

Learning Objective:

- Upon studying this paper, the students will be able to answer CSIR-NET questions in Physical Chemistry.

Course Outcomes:

The Learners will be able to

1. Apply quantum chemistry to solve Schrödinger wave equation for one, two- and three-dimensional boxes and for hydrogen and helium atoms, apply the approximation methods to single and multi-electron systems, and discuss the concepts of atomic structure, spectroscopy and apply term symbols to many electron systems.
2. Elaborate Huckel theory to conjugated systems, concepts of symmetry in molecular vibrations, chemical bonding and electronic transitions.
3. Compile the concepts of chemical kinetics and enzyme kinetics, describe the concepts of statistical thermodynamics and apply the partition function to model systems.
4. Relate the concepts of electrochemistry, explain the kinetics of reactions in solutions, acid-base catalysis and surface reactions.
5. Illustrate the theory and properties of colloids, mechanism of heterogeneous catalysis and structure of solids, discuss the kinetics of polymerization, and data analysis.

CO	PSO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

CO	PO					
	1	2	3	4	5	6
CO1	H	H	H	H	H	H
CO2	H	H	H	H	H	H
CO3	H	H	H	H	H	H
CO4	H	H	H	H	H	H
CO5	H	H	H	H	H	H

H-High (3), M-Moderate (2), L-Low (1)

Unit I

1.1. Basic principles of quantum mechanics, postulates, operator algebra, exactly-solvable systems. (K1, K2, K3 & K4)

1.2. Particle-in-a-box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals, orbital and spin angular momenta, tunneling. (K1, K2, K3 & K4)

1.3. Approximation methods of quantum mechanics: Variational principle for multi electron systems. (K1, K2, K3, K4 & K5)

1.4. Perturbation method and its application to multielectron systems. (K1, K2, K3 & K4)

1.5 Atomic structure and spectroscopy. (K1, K2, K3 & K4)

1.6 Term symbols - many-electron systems and antisymmetry principle. (K1, K2, K3, K4 & K5)

Unit II

2.1 Chemical bonding in diatomics, elementary concepts of MO and VB theories. (K1, K2, K3 & K4)

2.2 Huckel theory for conjugated π-electron systems. (K1, K2, K3, K4 & K5)

2.3 Chemical applications of group theory, symmetry elements, point groups, character tables, selection rules. (K1, K2, K3 & K4)

2.4 Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules. (K1, K2, K3 & K4)

2.5 Electronic spectra - principle and application. (K1, K2, K3, K4 & K5)

2.6 IR and Raman spectra - selection rules, basic principles of magnetic resonance. (K1, K2, K3 & K4)

Unit III

3.1 Chemical thermodynamics: Laws, state and path functions and their applications, thermodynamic description of various types of processes. (K1, K2, K3 & K4)

3.2 Maxwell's relations, spontaneity and equilibria, temperature and pressure dependence of thermodynamic quantities. (K1, K2, K3, K4 & K5)

3.3 Le Chatelier's principle, elementary description of phase transitions, phase equilibria and phase rule. (K1, K2, K3 & K4)

3.4 Thermodynamics of ideal and non-ideal gases, and solutions. (K1, K2, K3 & K4)

3.5 Statistical thermodynamics: Boltzmann distribution and kinetic theory of gases. (K1, K2, K3 & K4)

3.6 Partition functions and their relation to thermodynamic quantities - calculations for model systems. (K1, K2, K3 & K4)

Unit IV

4.1 Electrochemistry: Nernst equation, redox systems, electrochemical cells, Debye-Huckel theory (K1, K2, K3 & K4)

4.2 Electrolytic conductance - Kohlrausch's law and its applications, ionic equilibria, conductometric and potentiometric titrations. (K1, K2, K3 & K4)

4.3 Chemical kinetics: Empirical rate laws and temperature dependence, complex reactions, steady state approximation, determination of reaction mechanisms. (K1, K2, K3 & K4)

4.4 Collision and transition state theories of rate constants, unimolecular reactions. (K1, K2, K3, K4 & K5)

4.5 Enzyme kinetics and salt effects. (K1, K2, K3 & K4)

4.6 Homogeneous catalysis and photochemical reactions. (K1, K2, K3 & K4)

Unit V

5.1 Colloids and surfaces: Stability and properties of colloids, isotherms and surface area. (K1, K2, K3 & K4)

5.2 Heterogeneous catalysis. (K1, K2, K3 & K4)

5.3 Solid state: Crystal structures, Bragg's law and applications, band structure of solids. (K1, K2, K3 & K4)

5.4 Polymer chemistry: Molar masses, kinetics of polymerization. (K1, K2, K3 & K4)

5.5 Data analysis: Mean and standard deviation, absolute and relative errors. (K1, K2 & K3)

5.6 Linear regression, covariance and correlation coefficient. (K1, K2, K3 & K4)

Reference Books:

1. J. E. Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper Collins, New York, 4th Edition, 1993.
2. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, John Wiley and Sons, 5th Edition, 1988.
3. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, WB Saunders Co., USA, 1977.
4. R. G. Frost and Pearson, Kinetics and Mechanism, Wiley, New York, First Reprint 1970.
5. Keith J. Laidler, Chemical Kinetics, Pearson Edition Company Pvt. Ltd., Third Edition, 2005.
6. P. W. Atkins, Physical Chemistry, Oxford University Press, 7th Edition, 2002.
7. J. Rajaram J. C. Kuriacose, Kinetics and Mechanisms of Chemical Transformations: Applications of Femto Chemistry, Mc Millan Publishers India Ltd., Reprint 2009.
8. V. R. Gowarikar, Viswanathan J. Sridhar, Polymer Science, Wiley Eastern, Reprint 2005.
9. F. W. Billmeyer, Textbook of Polymer Science, Wiley Inter Science, 3rd Edition. 2005.
10. K. V. Raman, Group Theory and Its Applications to Chemistry, Tata McGraw-Hill Publishing Company Ltd., Reprint 2004.
11. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishing Co., Reprint 2005.
12. F. A. Cotton, Group Theory and Its Applications to Chemistry, John Wiley & Sons (Asia) Pvt. Ltd., Singapore, 2004.
13. A. Salahuddin Kunju and G. Krishnan, Group theory and its Applications in Chemistry, Asoke K. Ghosh, PHI Learning Pvt. Ltd., New Delhi, 2010.

OER:

1. https://www.examrace.com/CSIR/CSIR-Free-Study-Material/CSIR-Chemical-Sciences/Chemistry/Physical-Chemistry/
2. https://www.chemistryabc.com/download/notes/csir-ugc-net-notes/
3. https://ocw.mit.edu/courses/chemistry/5-61-physical-chemistry-fall-2007/lecture-notes/