Central University of Punjab



Course Structure and Syllabus

M.Sc. Chemistry (Specialization: Applied

Chemistry)

Session: 2021-23

Department of Chemistry School of Basic Sciences

Graduate Attributes for M.Sc. Chemistry (Specialization: Applied Chemistry)

The Graduates will be able to identify various aspects of chemicals and their application in consumer products and industrial set-up. They have comprehensive knowledge and understanding of their subject, for application in a multidisciplinary environment. They will be effective in quality control and optimization in the industrial environment, applying critical creative and evidence based thinking to conceive innovative responses to policy, economics and project management.

The graduates will engage in professional behaviour, communicate well in the group as well as in other groups/institutions, have entrepreneurial potential. They will be able to take leadership roles in their occupations, careers and community with ethical behaviour. They will be able to contribute to a multicultural, IT revolutionized and sustainable society/policy as global citizens.

Semester I

S. No	Paper Code	Course Title Cours e Type		L	Т	P	C r
1	CHM.506	Fundamental Biology *	CF	2	1	0	1
1	CHM.507	Fundamental Mathematics**	Fundamental Mathematics** CF		1	0	3
2	CHM.509	Inorganic Chemistry – I	С	3	0	0	3
3	CHM.510	Organic Chemistry – I	С	3	0	o	3
4	CHM.511	Physical Chemistry – I	С	3	0	0	3
5	CHM.512	Quantum Chemistry	CF	3	0	0	3
6	CHM.513 Inorganic Chemistry (Practical) SB		0	0	4	2	
7	CHM.514	Organic Chemistry (Practical) SB		0	0	4	2
8	XXX.XXX	Interdisciplinary Course# ID		2	0	0	2
	Total					8	2 1
Inte	rdisciplinar	y Course Offered by Department	for othe	r De	partmo	ents	,
9	CHM.515	Basics perspective in Inorganic Chemistry	ID	2	0	0	2
10	CHM.516	Introduction to Green Chemistry and Sustainability	ID	2	0	0	2
11	CHM.517	Chemistry of Nanomaterials and Fabrication	ID	2	0	0	2
12	CHM.518	General Laboratory Practices ID		2	0	0	2
13	CHM.519	Chemicals of Everyday Life ID		2	0	0	2
14	CHM.605	Chemistry of Drug Design and Synthesis		2	0	0	2

^{*}Student having studied mathematics in B.Sc. need to opt this course

** Student having studied life sciences in B.Sc. need to opt this course

To be opted from other departments at the start of the Semester with prior consent of course coordinator and HoD.

C: Core Course, CF: Compulsory Foundation, SB: Skill Based, ID: Interdisciplinary Course.

L: Lectures T: Tutorial P: Practical Cr: Credits

Semester II

S N o	Paper Code	Course Title	Cours e Type	L	Т	P	C r
1	CHM.521	Inorganic Chemistry – II	3	0	0	3	
2	CHM.522	Organic Chemistry – II	С	3	0	0	3
3	CHM.523	Physical Chemistry – II	С	3	0	0	3
4	CHM.524	Spectroscopic Analysis	С	3	0	0	3
5	CHM.525	Molecular Spectroscopy	С	3	0	0	3
6	CHM.527	Physical Chemistry (Practical) SB		0	0	4	2
7	CHM.529	Computational and Structural Chemistry (Practical)	SB	0	0	4	2
7	CHM.530	Entrepreneurship	CF	1	0	0	1
8	XXX	Value Added Course*	VAC	2	0	0	2
То	tal Credit (F	Iours)		18	0	8	2 2
	Value Add	ed Course offered by Department t	o other I	Depa	rtme	nts	
1 0	CHM.528	Protein Chemistry	VAC	2	0	0	2
11 ·	CHM.503	Biological Inorganic Chemistry	VAC	2	0	0	2
1 2.	CHM.505	Spectroscopic and Chromatographic Techniques	VAC	2	0	0	2

^{*} To be opted at the start of the Semester and would be run at the university level with prior consent of course coordinator/HoD.

C: Core Course, CF: Compulsory Foundation, SB: Skill Based, VAC: Value-added Course

L: Lectures T: Tutorial P: Practical Cr: Credits

Semester III

S. No	Paper Code	Course Title Cours e Type			Т	P	Cr
1	CAC.551	Advanced Applied Chemistry Practical	SB	0	0	4	2
2	CAC.553	Quality Control in Laboratory and Manufacturing	С	3	0	0	3
3	CAC.585	Pharmaceutical Products	С	3	0	0	3
4	CHM.559	Advanced Logics in Chemistry	DEC	2	0	0	2
5	CAC.600	Research Proposal	SB	0	0	8	4
Opt	Any Three (03) Elective Course/ MOOC	•	9	0	0	9
6	CHM.551	Inorganic Chemistry-III	DE	3	0	0	3
7	CHM.552	Organic Chemistry-III	DE	3	0	0	3
8	CHM.553	Bioinorganic and Biophysical Chemistry	DE	3	0	0	3
9	CAC.554	Applied Electrochemistry	DE	3	0	0	3
10	CAC.559	Organic Synthesis and Catalysis	DE	3	0	0	3
11	CAC.560	Environmental Chemistry	DE	3	0	0	3
12	CAC.571	Applied Polymer Chemistry	DE	3	0	0	3
13	CAC.572	Green and Industrial Organic Chemistry	DE	3	0	0	3
14	CAC.573	Industrial Inorganic Chemistry	DE	3	0	0	3
15	CAC.575	Dyes and Pigments	DE		o	0	3
16	CAC.576	Petroleum Chemistry	DE	3	o	0	3
17	CAC.577	Advance Instrumental Methods	DE	3	o	0	3
18	CAC.581	Applied Material Chemistry	DE	3	o	0	3
19	FST.506	Food Chemistry	DE	3	0	0	3

20	BCH.509	Bioanalytical Techniques	DE	3	0	0	3
	Total				0	12	23

C: Core Course, SB: Skill-Based Course, DEC: Discipline-Enrichment Course, DE:

Elective Courses

L: Lectures T: Tutorial P: Practical Cr: Credits

Semester-IV

S. No	Paper Code	Course Title	Course Type	L	Т	P	Cr
1	CAC.600	Dissertation	SB	0	0	40	20
		Total		0	0	40	20

SC: Skill Based Course

L: Lectures T: Tutorial P: Practical Cr: Credits

Examination Pattern

Core, Discipline Elective, Compulsory Foundation, Value Added and Interdisciplinary Courses			Discipline Enrichment Course		Entrepreneurship Course	
	Mark s	Evaluation Methods	Mark s	Evaluation Methods	Mar ks	Evaluation Methods
Internal Assessment	25	Various	-	-	-	-
Mid- semester test (MST)	25	Subjective	50	Objective	25	Objective
End- semester test (EST)	50	Subjective (70%) Objective (30%)	50	Objective	25	Subjective

The **objective type evaluation** will include one word answers, fill-in the blank, sentence completion, true/false, MCQs', matching, analogies, rating and checklists.

The **subjective type evaluation will** include a very short answer (1–2 lines), short answer (one paragraph), essay type with restricted response, and essay type with extended response.

Dissertation Evaluation:

Dissertation Proposal (Third Semester)			Dissertation (Fourth Semester)			
	M ar ks	Evaluation Method		M ar ks	Evaluation Method	
Supervisor	50	Dissertation proposal and presentation	Supervisor	50	Continuous assessment (regularity in work, mid-term evaluation) dissertation report, presentation, final viva-voce	

HoD and senior- most faculty of the department	_	Dissertation proposal and presentation	External expert, HoD and senior- most faculty of the department		Dissertation report (30), presentation (10), final viva-voce (10)
--	---	--	---	--	---

Internal Assessment Methods: Surprise Tests, in-depth interview, unstructured interview, Jigsaw method, Think-Pair Share, Students Teams Achievement Division (STAD), Rubrics, portfolios, case based evaluation, video based evaluation, Kahoot, Padlet, Directed paraphrasing, Approximate analogies, one sentence summary, Pros and cons grid, student generated questions, case analysis, simulated problem solving, media assisted evaluation, Application cards, Minute paper, open book techniques, classroom assignments, home assignments, term paper.

L	Т	P	Cr
2	1	0	3

Course Title: Fundamental Biology (Non-medical group)

Paper Code: CHM.506 Total Contact Hours: 30

Learning Outcome: After this course completion, students will be able to

- Interpret molecular structure and interactions present in proteins, nucleic acids, carbohydrates and lipids.
- Demonstrate the organization and working principles of various components present in the living cell.
- Apply the knowledge of Physical principles of structure, function, and folding of biomolecules.

Unit 1 7 Hours

Introduction: Cell structure and functions, thermodynamics and kinetics of biological processes, ATP. Role of water in life, pH, Acidic and basic buffers, Biological buffers, solution equilibria, Henderson-Hasselbalch equation, Hofmeister series, Chaotropic and kosmotropic ions/co-solvents.

Peer discussion on role of buffers in Biological system and stability of drug formulations

Unit 2 8 Hours

Amino Acids and Peptides: Classification and properties of amino acids, peptide and polypeptides, primary structures, structure of peptide bond, synthesis of peptides, different protecting groups in peptide chemistry, N-terminal, C-terminal and sequence determination.

Carbohydrates: Biologically important monosaccharides, disaccharides and polysaccharides and glycoproteins.

Importance of peptides and carbohydrates in the context of biology through peer learning

Unit 3 7 Hours

Proteins: Secondary structure of proteins with emphasize on supramolecular characteristics of alpha-helix, beta-helix, tertiary structure of protein-folding, quaternary structure of protein, in-vivo and in-vitro protein folding, protein misfolding and conformational diseases.

Secondary, tertiary and quaternary structure of Proteins: Classroom debate

Unit 4 8 Hours

Nucleic Acids: Purine and pyrimidine bases, nucleotides, nucleosides, base pairing *via* H-bonding, structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA, different types of RNA and their functions, the chemical basis for heredity.

Lipids: Lipid classification, lipid bilayers, lipoproteins-composition. High density (HDL) and low-density (LDL) lipoproteins and function.

3D structures of DNA, RNA: Peer discussion

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

Suggested Readings

- 1. Voet, D., Voet, J. G., and Pratt, C. W. (2018). *Principle of Biochemistry*. John Wiley and Sons.
- 2. Berg, J. M., Stryer, L., and Tymoczko, J. L. (2015). Stryer Biochemie. Springer-Verlag.
- 3. Garrett, R. H., and Grisham, C. M. (2013). *Biochemistry*, Brooks/Cole, Cengage Learning.
- 4. Conn, E., and Stumpf, P. (2009). *Outlines of Biochemistry*. John Wiley and Sons.
- 5. Frenkel-Pinter, M., Samanta, M., Ashkenasy, G., Leman, L.J. Prebiotic Peptides: Molecular Hubs in the Origin of Life, *Chem. Rev.* 2020, 120, 11, 4707–4765.
- 6. Shivatare, S. S., Wong, C-H. Synthetic Carbohydrate Chemistry and Translational Medicine, J. Org. Chem. 2020, 85, 24, 15780–15800

L	Т	P	Cr
2	1	0	3

Course Title: Fundamental Mathematics

Paper Code: CHM.507 Total Contact Hours: 45

Learning Outcome: The students will be able to

- Demonstrate and apply the various mathematical operations including matrix operations, differentiation, integration, complex, quadratic and differential equations for common problems in chemistry.
- Demonstrate and apply the statistical methods in experimental evaluations in chemistry.

Unit 1 11 Hours

Trigonometric functions: Trigonometric operations for sum and differences of angles, addition and subtraction formulas.

Algebra: Polynomial equations and their solutions: binomial theorem and expansion. Common series and expansions used in chemistry.

Complex Algebra: Complex numbers, the graphical interpretation of complex numbers, characterizations of the exponential function, the trigonometric functions of complex argument (e^{iq}, e^{-iq}).

Peer discussion on the functions and their characteristics graphical behaviours

Unit 2 12 Hours

Differential Calculus

Functions, limits, continuity, first principle of differentiation, basic rules of differentiation, maxima and minima, exact and inexact differentials, partial differentiation, application to solution of potential energy, van der Waals radii, velocity and Boltzmann distribution.

Matrix Algebra: Addition and multiplication; inverse, adjoint and transpose of matrices, matrix equation, Introduction to vector spaces, matrix Eigenvalues and Eigenvectors, diagonalization, determinants (examples from Huckel theory).

Problem solving approach and revisiting problems in chemistry at undergraduate level quantum chemistry on matrix based solutions.

Unit 3 11 Hours

Integral Calculus

Basic rules for integration, integration by parts, partial fraction and substitution, definite integrals, evaluation of definite and some standard integrals related to chemistry

Elementary Differential Equations: Variables-separable and exact, first-order differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, quantum chemistry, etc. solutions of differential equations by the power series method, spherical harmonics, second order differential equations and their solutions.

Brainstorming and Problem solving approach for integral calculus and differential equations in chemistry related problems

Unit 4 11 Hours

Basic Statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness. Confidence interval, Errors, Levels of significance, Hypothesis testing.

Comparing means of two or more groups: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), χ^2 test.

Regression and correlation: Standard errors of regression coefficients, Comparing two regression lines.

Peer discussion of the significance of linear regression to chemistry and hypothesis testing.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Anderson, J. M. (2012) Mathematics for Quantum Chemistry, Dover Publications.
- 2. Francis, P. G.(2012) Mathematics for Chemists, Springer Netherlands.
- 3. Dickinson, F., McKinley, A.,(2021) Introduction to Contextual Maths in Chemistry, Royal Society of Chemistry.
- 4. Martin Cockett, Graham Doggett (2012) Maths for Chemists, Royal Society of Chemistry.
- 5. Hotta, S., (2019) Mathematical Physical Chemistry: Practical and Intuitive Methodology, Springer Press.
- 6. Barrante, J. R. (2016) Applied Mathematics for Physical Chemistry, 3rd Ed., Waveland Press.
- 7. Steiner, E. (2008). The Chemistry Maths Book. Oxford University Press.
- 8. Doggett, G., and Sutcliffe, B. T. (1995). *Mathematics for Chemistry*. Longman Pub Group.
- 9. Daniels, F. (2003). *Mathematical Preparation for Physical Chemistry*. McGraw Hill Publishers.
- 10. Tebbutt, P. (1998). Basic Mathematics for Chemists. Chichester: Wiley.

- 11. Skoog, D. A., Holler, F. J., and Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage learning
- 12. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.

L	Т	P	Cr
3	0	0	3

Course Title: Inorganic Chemistry - I

Paper Code: CHM.509 Total Contact Hours: 45

Learning Outcome: On completion of this course the student's will able to

- Reaction mechanism, formation constant and stability of the coordination complexes.
- Interpret the electronic properties.
- Interpret the magnetic properties

Unit 1 Hours

Metal-Ligand Equilibria in Solution: Stepwise and overall formation constant and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of formation constants by spectrophotometry and potentiometric (pH) methods.

Group Discussion among the students on the stability of metal complex formation

Unit 2 Hours

Reaction Mechanisms of Transition Metal Complexes: Introduction, potential energy diagram and reactivity of metal complexes, ligand substitution reactions, labile and inert metal complexes, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reaction, substitution reactions in square planar complexes, trans effect, mechanism of the substitution reaction reactions

without metal ligand bond cleavage, electron transfer processes outer and inner sphere.

Demonstration of reactions mechanism of metal complexes.

Unit 3 15 Hours

Electronic Absorption spectra of Metal Complexes: Ligand field theory, nephelauxetic effect, Jahn-Teller effects, spin orbital (LS) coupling, LS and J-J coupling schemes, determination of all the spectroscopic terms of p^n , d^n , f^n ions, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, spin orbit coupling parameters (λ) energy separation between different j states, the effect of octahedral and tetrahedral fields on S, P, D and F terms. selection rules of electronic transitions, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, spectrochemical series, band intensities, factors influencing band widths.

Classroom discussion on interpretation of LS coupling and various energy level diagrams through brainstorming

Unit 4
Hours

Magnetic properties: magnetic properties of transition metal complexes, effects of L-S coupling on magnetic properties, quenching of orbital angular momentum by crystal fields in complexes in terms of splitting, temperature independent paramagnetism (TIP).

Hand on experience of metal complexes for magnetic properties by using Gouy's Balance.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

- 1. Cotton, F. A., and Wilkinson, G., Murillo, C. A., Bochmann, M.(1999). *Advanced Inorganic Chemistry* (6th Edition). New York: Wiley.
- 2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity.* Pearson Education India.
- 3. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
- 4. Miessler, G. L. and Tarr, D. A. (2011) *Inorganic Chemistry*, Pearson Education.
- 5. Atkins, P. (2010). Shriver and Atkins' Inorganic Chemistry. Oxford University Press, USA.
- 6. Dutta, R. L., and Syamal, A. (1993). *Elements of Magnetochemistry*. Affiliated East-West Press.
- 7. Drago, R. S. (1992) *Physical Methods for Chemists*. Saunders College Publishing.

- 8. Lee, J. D. Concise Inorganic Chemistry: Fifth Edition (2012). Elsevier.
- 9. Kent, B. Inorganic Chemistry: Reactions, Structures and Mechanisms (12 June 2019), NY Research Press.
- 10. Close, D. Principles of Inorganic Chemistry (19 June 2019), Larsen and Keller Education

L	Т	P	Cr
3	0	0	3

Course Title: Organic Chemistry-I

Paper Code: CHM.510 Total Contact Hours: 45

Learning Outcome: After the completion of the course students will be able to

- Identify various methods and intermediate species involved while determining the mechanism of organic reactions.
- Examine the mechanistic and synthetic aspects of nucleophilic and electrophilic substitution reactions.
- Explore the implications of enolate chemistry for the synthesis of various molecules.

Unit 1 11Hours

Reaction mechanism, structure and reactivity: Classification and determination of reaction mechanisms, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, methods of determining mechanisms, isotope effects, effect of structure on reactivity: Hammett equation, Taft equation.

Reactive intermediates: Generation, structure and reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzynes. Neighbouring group participation, classical and non-classical carbocations, phenonium ions and norbornyl system.

Aromaticity: Aromaticity in benzenoid and non-benzenoid compounds, antiaromaticity, homoaromatic compounds.

Peer Discussion on stability of the intermediates in the presence of different substituents (electron-withdrawing and electron releasing)

Classroom discussion on various tools used for the determination of reaction mechanism

Unit 2

11Hours

Aliphatic nucleophilic substitution reaction: The S_N^2 , S_N^1 , mixed S_N^2 and S_N^1 , the S_N^1 mechanism. Energy profile diagram, nucleophilic substitution at an allylic, aliphatic and vinylic carbon reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, effect of solvent in substitution reaction, competition between S_N^2 and S_N^1 mechanisms, ion pair theory.

Aromatic nucleophilic substitution: The S_N^{Ar} , bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, *ortho/para* ratio, *ipso* attack, orientation in other ring systems.

Demonstration of substitution reactions with the help of ball and stick models Peer discussion on the role of substituents in electrophilic and nucleophilic substitution reaction

Unit 3 11Hours

Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

Demonstration of elimination reactions with the help of ball and stick models Addition of different reactive intermediates to alkenes and alkynes through peer learning

Unit 4 12Hours

Addition to carbon-hetero multiple bonds: Structure and reactivity of carbonyl group towards nucleophilic addition: addition of CN, ROH, RSH, H₂O, hydride ion, ammonia derivatives, LiAlH₄, NaBH₄, organozinc and organolithium reagents to carbonyl and conjugated carbonyl compounds, Arndt-Eistert synthesis. Mechanism of condensation reactions involving enolates: Aldol, Knoevenagel, Claisen, Dieckmann, Mannich, Benzoin, Perkin and Stobbe reactions. Carboxylic acids and derivatives, hydrolysis of esters and amides, ammonolysis of esters.

Peer discussion of the mechanism of nucleophilic additions to carbonyl, nitrile, thiocarbonyl, carboxylic acids, esters and amides

Mechanistic interpretation of C-C, C-N and C-O bond formation reactions through brainstorming

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. (2012) Organic Chemistry, Oxford University Press.
- 2. Finar, I. L. (1996). *Textbook of Organic Chemistry*. ELBS, Pearson Education UK.
- 3. Yadav, L. D. S., Singh, J., and Singh, J. (2017). Organic Synthesis, Pragati Prakashan, India.
- 4. Norman, R. O. C., and Coxon, J. M. (1993). Principle of Organic Synthesis, CRC Press; 3rd edition.
- 5. McMurry, J. (1996). Organic Chemistry, Brooks. Cole, New York, 657.
- 6. Smith, M. B., and March, J. (2013). March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure. John Wiley and Sons.
- 7. Ahluwalia, V. K., and Parashar, R. K. (2011). *Organic Reaction Mechanisms*. Narosa Publishing House (P) Ltd.
- 8. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.
- 9. Bansal R. K. (2010) *Organic Reaction Mechanism.* New Age International (P) Ltd.
- 10. Kalsi, P. S. (2010) Organic Reactions and Their Mechanisms. New Age International, New Delhi.
- 11. Lowry, T. H. and Richardson K. S. (1998) *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., New York.
- 12. Morrison, R.T. and Boyd, R.N. (2011) *Organic Chemistry*, Prentice-Hall of India.
- 13. Mukherjee, S. M. and Singh, S. P. (2009) *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi.
- 14. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A. (2013) *Organic Chemistry*. John Wiley and Sons, Inc.
- 15. Sykes, P. A. (1997) *Guide Book to Mechanism in Organic Chemistry*, Prentice Hall.
- 16. Stein, T. H., Vasiliu, M., Arduengo, A. J. Lewis Acidity and Basicity: Another Measure of Carbene Reactivity, *J. Phys. Chem. A* 2020, 124, 29, 6096–6103.
- 17. Morisaki, K., Morimoto, H., Ohshima, T. Recent Progress on Catalytic Addition Reactions to *N*-Unsubstituted Imines, *ACS Catal.* 2020, 10, 12, 6924–6951.

L	Т	P	Cr

3	0	0	3

Course Title: Physical Chemistry-I

Paper Code: CHM.511 Total Contact Hours: 45

Learning Outcome: After the completion of the course students will be able

to

- Interpret classical thermodynamics and thermodynamic phenomenon in a chemical system
- Explore the solutions of nonelectrolytes and electrolytes and draw the phase transition of different system
- Explain the statistical aspects of thermodynamics
- Apprehend and apply partition function in the deduction of thermodynamic properties of chemical systems.
- Apprehend and apply Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics according to the thermodynamic system.

Unit 1 Hours

Partial Molar Properties and Fugacity: Partial molar properties. Chemical potential of a perfect gas, dependence of chemical potential on temperature and pressure, Gibbs-Duhem equation, fugacity, its importance and determination.

Thermodynamics of Simple Mixtures: Thermodynamic functions for mixing of perfect gases. Chemical potential of liquids. Raoult's law, thermodynamic functions for mixing of liquids (ideal solutions only). Real solutions and activities. Activity coefficient; determination of activity and activity coefficients.

Problem solving approach with defining the dynamic chemical process with the evaluation of chemical potential and activity.

Unit 2 Hours

Colligative Properties: Colligative properties of solutions, such as osmotic pressure, depression of the freezing point and elevation of the boiling point. **Phase transition:** Phase rule, water, CO₂ phase transition, binary and ternary component phase transitions. Clausius-Clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

Problem solving on colligative properties and phase equilibria thermodynamics

Unit 3 12 Hours

Statistical Thermodynamics: Statistical concepts and examples, Thermodynamic probability and entropy, Partition function, molar partition function, thermodynamic properties in term of molecular partition function for monoatomic gases, rotational, translational, vibrational and electronic partition functions for diatomic molecules, calculation of equilibrium constants in term of partition function.

Partition function and its correlation to classical thermodynamic evaluation through brainstorming session and peer learning

Unit 4 Hours

Theories of Statistical Thermodynamics: Concept of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Difference between Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Applications of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics., Monoatomic solids, theories of specific heat for solids.

Demonstrating application of various statistical thermodynamic theories and Debye theory for heat capacity.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Kapoor, K. L. (2011) *Textbook of Physical Chemistry*.3/5, Macmillan Publishers.
- 2. Atkins, P., De Paula, J. and Keeler, J. (2018) Atkins' Physical Chemistry. 11th ed. Oxford University Press.
- 3. McQuarrie, D. A. and Simon, J. D. (2019) Physical Chemistry: A Molecular Approach. Viva Books.
- 4. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2004) *Physical Chemistry*. Wiley-Interscience Publication.
- 5. Engel, T., Reid, P. and Hehre, W. (2012) *Physical Chemistry*. Pearson Education.
- 6. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company.
- 7. Rastogi, R. P. and Mishra, R. R. (2013) An Introduction to Chemical Thermodynamics. Vikas Publishing
- 8. Rajaram, J. and Kuriacose, J. C. (2013) Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics. Pearson Education.
- 9. Nash, L. K. (2012) *Elements of Statistical Thermodynamics*. Dover Publication Inc.

- 10. Laurendeau, N. M. (2005) Statistical Thermodynamics: Fundamentals and Applications. Cambridge University Press.
- 11. Hill, T. L. (1986) *An Introduction to Statistical Thermodynamics*. Dover Publications Inc.
- 12. Yu, T. H. (2020) Teaching Thermodynamics with the Quantum Volume J. Chem. Educ., 97 (3), 736-740 DOI: 10.1021/acs.jchemed.9b00742
- 13. Fitzgerald, J.P., Ferrante, R. F., Brown, M., and Cabarrus, J. (2020) Relating ΔHvap of Organic Liquids to Intermolecular Forces: Simple Modifications of a Classic General Chemistry Experiment J. Chem. Educ., 97 (5), 1406–1410 DOI: 10.1021/acs.jchemed.0c00163
- 14. Nelson, K. A., Bawendi, M. (2008) https://ocw.mit.edu/courses/chemistry/5-60-thermodynamics-kinetics-spring-2008/video-lectures.
- 15. Bjorn Joos, B., Van Bael, M. K. and Hardy, A. T. (2020) Construction of a Room-Temperature Eutectic Binary Phase Diagram by Use of Differential Scanning Calorimetry. *J. Chem. Educ.*, 97 (8), 2265-2272. DOI: 10.1021/acs.jchemed.0c00204
- 16. Bhattacharyya, D. and Dawlaty, J. M. (2019) Teaching Entropy from Phase Space Perspective: Connecting the Statistical and Thermodynamic Views Using a Simple One-Dimensional Model *J. Chem. Educ.*, 96 (10), 2208–2216. DOI: 10.1021/acs.jchemed.9b00134
- 17. Halpern A. M. and Marzzacco, C. J. (2018) Using the Principles of Classical and Statistical Thermodynamics to Calculate the Melting and Boiling Points, Enthalpies and Entropies of Fusion and Vaporization of Water, and the Freezing Point Depression and Boiling Point Elevation of Ideal and Nonideal Aqueous Solutions, *J. Chem. Educ.*, 95(12), 2205–2211. DOI: 10.1021/acs.jchemed.8b00561
- 18. Halpern A. M. and Marzzacco, C. J. (2018) Constructing the Phase Diagram of a Single-Component System Using Fundamental Principles of Thermodynamics and Statistical Mechanics: A Spreadsheet-Based Learning Experience for Students. *J. Chem. Educ.*, 95 (12), 2197-2204. DOI: 10.1021/acs.jchemed.8b00560

L	Т	P	Cr
3	0	0	3

Course Title: Quantum Chemistry

Paper Code: CHM.512 Total Contact Hours: 45

Learning Outcome: The students will be able to

- Interpret and solve the Schrodinger equation for various systems, particle in a boundary model, Electronic and Hamiltonian operators for molecules.
- Explain the quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
- Relate the Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle with the atomic and molecular phenomena.

Unit 1

11Hours

Fundamental Background: Review of essential mathematical concepts required for quantum chemistry, Postulates of quantum mechanics, Eigen values and Eigen functions, operators, Schrodinger equation.

Problem solving approach to determine Eigen values and Eigen function using corresponding operator and Schrodinger equation.

Unit 2

11Hours

Translational, Rotational and Vibrational Motions: - Free particle and particle in a box and its application (*i.e.*, quantum tunneling effect), one-dimensional harmonic oscillator and rigid rotor, particle in a ring, particle on a sphere, hydrogen like atoms

Variation Methods: The variation theorem and its application, linear variation principle.

Brainstorming on defining and solving Schrodinger equation for different systems like particle in a box, rigid rotator, simple harmonic oscillator, hydrogen like atom.

Unit 3

12Hours

Angular Momentum: Ordinary angular momentum, generalized angular momentum, Eigen functions and Eigen values for angular momentum, Ladder operator, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle, Slater determinant wave functions.

Electronic Structure of Atoms: Electronic configuration, term symbols and spectroscopic states, Russell-Saunders terms and J-J coupling schemes, Magnetic effects: spin-orbit coupling and Zeeman splitting.

Understanding multi-electron atom quantum evaluation through peer discussion and brainstorming session.

Unit 4 11Hours

Born-Oppenheimer Approximation: LCAO-MO and VB treatments of the H₂⁺ and H₂, Shape of molecules, Hybridization and valence MOs of H₂O and NH₃. Determination of bond angle in sp³, sp² and sp, Huckel Theory of acyclic and cyclic conjugated systems, Bond order and charge density

Application of pi-HMO theory for acyclic and cyclic conjugated organic systems through peer learning. Application of MOT and VBT for H_2 and H_2 ⁺ system through demonstration.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming.

Suggested Readings

- 1. Levine, I.N. (2014) Quantum Chemistry. 7th ed. Pearson Education Inc.
- 2. Chandra, A.K. (2017) *Introductory Quantum Chemistry*. 4th ed. Tata Mcgraw-Hill.
- 3. McQuarrie, D. A. and Simon, J. D. (1998) Physical Chemistry: A Molecular Approach. Viva Books.
- 4. Prasad, R.K., (2009) Quantum Chemistry. 4th Ed. New Age Science.
- 5. Murrell, J.N., Kettle S.F.A. and Tedder, J. M. (1965) *Valence Theory*. John Wiley Publishers.
- 6. Lowe, J. P. and Peterson, K., (2006). *Quantum Chemistry*. Academic Press.
- 7. Atkins, P., and Friedman, R. (2011). *Molecular Quantum Mechanics*, 5th edition, Oxford university press.
- 8. Drennan, C., Taylor, E. V., (2008) https://ocw.mit.edu/courses/chemistry/5-111-principles-of-chemical-science-fall-2008/index.htm
- 9. Griffin, R. G., Voorhis, T. V. (2007) https://ocw.mit.edu/courses/chemistry/5-111-principles-of-chemical-science-fall-2008/index.htm

L	Т	P	Cr
0	0	4	2

Course Title: Practical Inorganic Chemistry

Paper Code: CHM.513 Contact Hours: 60 h

Learning Outcome: The students will be able to

• perform volumetric and gravimetric analysis of cations and anions within reaction mixtures.

• Standardize and titrate various inorganic compounds.

Experiments:

Introduction to good laboratory practices in chemistry. Gravimetric Estimation

- 1. Determination of Ba²⁺ as its sulphate/chromate.
- 2. Estimation of lead as its lead sulfate.
- 3. Estimation of Nickel (II) as its nickel dimethyl glyoximate.
- 4. Estimation of Cu²⁺as cuprous thiocyanate.

Precipitation Titrations

- 1. AgNO₃ standardization by Mohr's method.
- 2. Volhard's method for Cl-determination.

Oxidation-Reduction Titrations

- 1. Standardization of KMnO₄with sodium oxalate and determination of Ca²⁺ ion.
- 2. Standardization of ceric sulphate with Mohr's salt and determination of Cu^{2+} , NO_2 and $C_2O_4^{-2}$ ions.
- 3. Standardization of $K_2Cr_2O_7$ with Fe^{2+} and determination of Fe^{3+} (Ferric alum)
- 4. Standardization of hypo solution with potassium iodate / $K_2Cr_2O_7$ and determination of available Cl_2 in bleaching powder, Sb^{3+} and Cu^{2+} .
- 5. Determination of hydrazine with KIO₃ titration.

Mode of Transactions: Demonstration, PPT, videos, Lecture cum demonstration

- 1. Pass, G. and Sutcliffe H. (1979) *Practical Inorganic Chemistry*. Chapman and Hall Ltd.
- 2. Jolly, W.L. (1961) Synthetic Inorganic Chemistry. Prentice Hall, Inc.
- 3. Nakamoto, K. (1997) Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B. John Wiley and Sons.
- 4. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M. J. K. (2000) *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Ltd.
- 5. Svehla, G. and Sivasankar, B. (1996) *Vogel's Qualitative Inorganic Analysis*. Pearson Education Ltd.
- 6. Skoog, D.A., Holler, F.J., and Crouch, S.R. (2007) *Principles of Instrumental Analysis*. Thomson Learning.

L	Т	P	Cr

0	0	4	2

Course Title: Practical Organic Chemistry

Paper Code: CHM.514 Total Contact Hours: 60

Learning Outcome: At the end of this course student will be able to

- Exercise good laboratory practices including safe handling of hazardous chemicals, laboratory glassware and equipment(s).
- Apply various experimental skills for purification, isolation and recrystallization of organic molecules.
- Analyze the progress of a given reaction on thin layer chromatography.

Experiments:

Safety and Handling of hazardous chemicals:

- (i) Good laboratory practices, handling and disposal of hazardous chemicals.
- (ii) Awareness about different types of glassware, heating devices, equipment(s), how to conduct organic reaction etc.

A. Techniques:

Chromatography: Thin layer chromatography (TLC): Monitoring the progress of chemical reactions, $R_{\rm f}$ values: identification of unknown organic compounds by comparing the $R_{\rm f}$ values with known standards. Column chromatography.

Purification Techniques: crystallization, distillation, sublimation.

Determination of melting point and mixed melting point.

- **B. Single Stage Synthesis**: Synthesis of compounds and their purification, aspects such as conversion, theoretical yield and percentage yield should be paid attention. (Attempt any six)
 - 1. Synthesis of chalcones via Claisen-Schmidt condensation.
 - 2. Reduction of benzophenone to benzhydral using NaBH₄.
 - 3. Conversion of benzaldehyde to cinnamic acid (Knoevenagel condensation)
 - 4. Conversion of benzaldehyde to dibenzylidene acetone (Aldol condensation)
 - 5. To prepare phenylpropene *via* dehydration of corresponding phenylpropanol.
 - 6. To prepare ethyl cinnamate *via* acid catalyzed esterification of cinnamic acid.
 - 7. Conversion of phthalic anhydride to phthalimide
 - 8. To synthesize arylidene analogue of Meldrum acid.
 - 9. Synthesis of alcohol *via* addition of Grignard reagent to an aldehyde.

Mode of Transactions: Demonstration, PPT, videos, Lecture cum demonstration

Suggested Readings

- 1. Harwood, L.M. and Moody, C.J. (1989) *Experimental Organic Chemistry*. Blackwell Scientific Publishers.
- 2. Vogel, A.I. (2003), 5th ed. *Textbook of Practical Organic Chemistry*. ELBS, Longman Group Ltd.
- 3. Mann, F.G. and Saunders, B.C. (2009) *Practical Organic Chemistry*. Orient Longman Pvt. Ltd.
- 4. Leonard, J. and Lygo, B. (1995) *Advanced Practical Organic Chemistry*. Chapman and Hall.
- 5. Armarego, W.L. and Chai, C. (2012) Purification of Laboratory Chemicals. Butterworth-Heinemann.
- 6. Young, J.A. (1991) Improving Safety in the Chemical Laboratory: A Practical Guide. Wiley Publishing.
- 7. Silver, J. Let Us Teach Proper Thin Layer Chromatography Technique, J. Chem. Educ. 2020, 97, 12, 4217–4219.
- 8. Tannya, R., Ibarra-Rivera, Delgado-Montemayor, c., Oviedo-Garza, F., Pérez-Meseguer, J., Rivas-Galindo, V. M., Waksman-Minsky, N., Pérez-López, A. (2020) Setting Up an Educational Column Chromatography Experiment from Home, J. Chem. Educ. 97, 9, 3055–3059.

L	Т	P	Cr
3	0	0	3

Course Title: Inorganic Chemistry-II

Paper Code: CHM.521 Total Contact Hours: 45

Learning Outcome: The students will able to

- Concepts to realize point group within chemical structure, character tables and projection operator techniques.
- Application of symmetry and group theory in spectroscopy.
- Structural properties of organometallic complexes and their uses.

Unit 1 10 Hours

Symmetry: Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination.

Basic discussion about types of symmetry and parameters to decide point groups in different molecules using of ball and stick models

Unit 2 10

Hours

Group theory: Determination of reducible and irreducible representations, character tables, construction of character tables for C_2v , C_3v , use of symmetry in obtaining symmetry of orbitals in molecules.

Group discussion to design the character tables of taking molecular examples and implication of ball and stick model tools.

Unit 3 15 Hours

Metal Complexes: Organic-transition metal chemistry, complexes with π -acceptor and σ -donor ligands, 18-electron and 16-electron rules, isolobal analogy, Synthesis and important reaction of metal carbonyls. Structure and bonding of metal carbonyls, metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligand and vibrational spectra of metal carbonyls for bonding and structure elucidation.

Discussion of various electron count rules and structural bonding parameters of organometallic compounds.

Unit 4 Hours

Inorganic cages: Metallocenes, metal cluster compounds, metal-metal bond, metal carbenes, carbonyl and non-carbonyl clusters, fluxional molecules, application of organometallic compounds as catalysts in organic synthesis.

Cage compounds of boron: boron cage compounds, boranes, carboranes and metallocene carboranes.

Peer discussion on Cage clusters formation rules via wede's and Mingos rules.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

- 1. Cotton, F. A., and Wilkinson, G. (1999). Advanced inorganic chemistry (4th edition). New York: Wiley.
- 2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic chemistry: principles of structure and reactivity.* Pearson Education India.
- 3. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
- 4. Lever, A.B.P. (1984) *Inorganic Electronic Spectroscopy*. Elsevier Science Publishers B.V.

- 5. Atkins, P. (2010). Shriver and Atkins' inorganic chemistry. Oxford University Press, USA.
- 6. Dutta, R. L., and Syamal, A. (1993). *Elements of magnetochemistry*. Affiliated East-West Press.
- 7. Lee, J. D. Concise Inorganic Chemistry: Fifth Edition (2012). Elsevier.
- 8. Kent, B. Inorganic Chemistry: Reactions, Structures and Mechanisms (12 June 2019), NY Research Press.
- 9. Close, D. Principles of Inorganic Chemistry (19 June 2019), Larsen and Keller Education

L	Т	P	Cr
3	0	0	3

Course Title: Organic Chemistry-II

Paper Code: CHM.522 Total Contact Hours: 45

Learning Outcome: The students will be able to

- Interpret and predict the energetically favoured conformation of cyclic and acyclic compounds, chirality and reactivity.
- Differentiate between thermally and photochemically driven pericyclic reactions and explain about their stereochemical aspects.
- Explore various molecular rearrangements in organic synthesis for the conversion of different functional group.

Unit 1 Hours

Stereochemistry: Chirality, projection formulae, configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, diastereoselectivity, D/L, R/S, E/Z and cis/trans configurational notations, threo and erythro isomers, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, conformational analysis of acyclic compounds and cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2, 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, effect of conformation on reactivity,

Demonstration of conformational and configurational analysis, projection formulae and topicity of the molecules with the help of ball and stick models. Ball and stick models of biphenyls, allenes and spiranes for chirality.

Unit 2

11 Hours

Photochemistry: Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency, photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Photochemistry of alkenes and enones, Paterno-Buchi reaction, Photoreduction, Di π – methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions.

Application of photochemical reactions in biologically important molecules through peer learning

Primary and secondary processes of photochemical reactions of carbonyl compounds and alkenes.

Unit 3 11 Hours

Pericyclic chemistry: Introduction, Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5- hexatriene, allyl cation, allyl radical, pentadienyl cation and pentadienyl radical.

Electrocyclic reactions: Conrotation and disrotation, 4n and 4n+2 systems. Woodward-Hoffmann rules. (i) Symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and correlation diagrams.

Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions and stereochemical aspects. Diels–Alder reaction. Woodward–Hoffmann Selection rules. Explanation for the mechanism by (i) Conservation of orbital symmetry and correlation diagrams (ii) FMO theory **Sigmatropic reactions**: [1,j] and [i,j] shifts; suprafacial and antarafacial, selection rules for [l, j] shifts; Cope and Claisen rearrangements; explanation for the mechanism by (i) symmetry properties of HOMO (ii) Introduction to cheletropic reactions and the explanation of mechanism by FMO theory.

Group project on the symmetry elements in FMO of 4npi and (4n+2)pi electron containing substrates

Quiz on FMO, correlation diagram and PMO approaches for pericyclic reactions

Unit4 Hours

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzillic acid, Favorskii, Neber, Beckmann, Hofmann, Curtius, Lossen, Schmidt, Carroll, Claisen, Cope, Gabriel-Colman, Smiles and Sommelet-Hauser rearrangements.

Selective Name Reactions: Ene/Alder-ene reaction, Dakin reaction, Reformatsky, Robinson annulation, Michael addition, Hofmann-Loffler Fretag, Chichibabin reaction.

Predicting the mechanistic pathways of rearrangement reactions through peer discussion

Application of important name reactions for bioactive molecule synthesis through brainstorming

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. (2012). *Organic Chemistry*. Oxford University Press.
- 2. Bansal, R. K. (2012). A Textbook of Organic Chemistry. New Age International.
- 3. Carey, F. A., and Sundberg, R. J. (2007). Advanced Organic Chemistry: Part A: Structure and Mechanisms. Springer Science and Business Media.
- 4. Kalsi, P. S. (2010). Stereochemistry Conformation and Mechanism. New Age International.
- 5. Eliel, E. L., and Wilen, S. H. (2008). *Stereochemistry of Organic Compounds*. John Wiley and Sons.
- 6. Carey, F. A., and Sundberg, R. J. (2007). Advanced Organic Chemistry: Part B. Springer Science and Business Media.
- 7. Finar, I. L. (1996). Textbook of Organic Chemistry. ELBS, Pearson Education UK.
- 8. Katritzky, A. R., Ramsden, C. A., Joule, J. A., and Zhdankin, V. V. (2010). *Handbook of Heterocyclic Chemistry*. Elsevier.
- 9. Norman, R.O.C. and Coxon, J.M. (1998). *Principles of Organic Synthesis*. Blackie Academic and Professional.
- 10. Fleming, I. (2015). *Pericyclic Reactions*. Oxford University Press.
- 11. Singh, J. (2005). *Photochemistry and Pericyclic Reactions*. New Age International.
- 12. McMurry, J. (1996). Organic Chemistry, Brooks. Cole, New York, 657.
- 13. Masson, G., Konig, B., Yoon, T. *Photochemical Synthesis*, Eur. J. Org. chem., 2020, 10, 1186–1585.
- 14. Elford, D., Lancaster, S. J., Jones, J. A. Stereoisomers, Not Stereo Enigmas: A Stereochemistry Escape Activity Incorporating Augmented and Immersive Virtual Reality, *J. Chem. Educ.* 2021, 98, 5, 1691–1704.

L	Т	P	Cr
3	0	0	3

Course Title: Physical Chemistry-II

Paper Code: CHM.523 Total Contact Hours: 45

Learning Outcome: The students will be able to

- Evaluate and predict the spontaneity of a redox processes in electrochemical systems
- Apply activity coefficient calculated from Debye-Huckel theory in real chemical solutions.
- Establish and evaluate the mechanism and kinetics for catalytic and photochemical reactions, homogenous and heterogeneous catalyzed reactions.
- Predict and establish the thermodynamic and kinetic aspects of adsorption characteristic of a material.
- Interpret the fast reaction monitoring for complex reactions.

Unit 1 12 Hours

Electrochemistry: Electrolytic conductance –Kohlrausch's Law, activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions, derivation of Debye-Huckel limiting law, extended Debye-Huckel law and conductometric titrations.

Electrochemical Cells: Nernst equation, redox systems, electrochemical cells, application of electrochemical cell, concentration cells with and without liquid junction, thermodynamics of reversible electrodes and reversible cells, potentiometric titration.

Understanding application of electrochemistry using classroom games activity. Expanding the understanding of conductance application using peer learning.

Unit 2 Hours

Reaction Kinetics: Introduction, rates of chemical reactions, complex reactions, steady state approximation, determination of mechanisms of chemical reactions, temperature dependence of rate constant, Arrhenius and Eyring equations and their applications, collision and transition state theories of rate constant, Kramers theory of reaction kinetics, treatment of unimolecular reactions, steric factor, ionic reactions: salt effect.

Understanding chemical kinetics and potential surface-reaction coordinate by hands on activity either as gaming, stochastic and molecular dynamic models.

Unit 3 Hours

Photochemical Reactions and Processes: Laws of photochemistry and kinetics of photochemical reactions, measurement of fluorescence and phosphorescence lifetimes and photoinduced electron transfer rates, photosensitization, quenching and photodimerization.

Fast Reaction Kinetics: Introduction to time-resolved techniques for absorption and emission measurements, relaxation method, study of kinetics of fast reactions by millisecond stopped-flow, nanosecond flash photolysis techniques, detection and kinetics of reactive intermediates,

Learning photochemical reaction kinetics through problem solving activities. Labon-chip based flow cell reactors using peer learning.

Unit 4 Hours

Adsorption: Adsorption of solids, Langmuir and Fredulich Isotherms, BET adsorption isotherm, Gibbs adsorption isotherm.

Catalysis: Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Michealis-Menten mechanism, Lineweaver-Burk Plot, competitive and non-competitive bindings, kinetics of catalytic reactions, application of enzyme catalysis.

Application and challenges in adsorption towards environmental and nanomaterial through peer learning. Enzyme binding and catalysis through inquiry guided and gaming based learning.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Laidler, K. J. (2003). Chemical Kinetics. Pearson Education Ltd.
- 2. Atkins, P., De Paula, J., and Keeler, J. (2018) Atkins' Physical Chemistry. Oxford University Press.
- 3. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2008) *Physical Chemistry*. Wiley-Interscience Publication.
- 4. Engel, T. and Reid, P. (2012). Thermodynamics, Statistical Thermodynamics, and Kinetics. Pearson Education.
- 5. Lakowicz, J. R. (2006). Principles of Fluorescence Spectroscopy. Springer.
- 6. Kapoor, K. L. (2011) *Text Book of Physical Chemistry*.3/5, Macmillan Publishers.
- 7. McQuarrie, D. A. and Simon, J. D. (2018) Physical Chemistry: A Molecular Approach. Viva Books.
- 8. Moore, J. W., and Pearson, R. G. (1981). *Kinetics and Mechanism*. John Wiley and Sons.
- 9. Puri, B.R., Sharma, L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company.

- 10. Krask, T. (2020) Establishing a Connection for Students between the Reacting System and the Particle Model with Games and Stochastic Simulations of the Arrhenius Equation, *J. Chem. Educ.*, 97 (7), 1951–1959 DOI: 10.1021/acs.jchemed.0c00081.
- 11. Changenet, P., Gustavsson, T., and Lampre, I. (2020) Introduction to Femtochemistry: Excited-State Proton Transfer from Pyranine to Water Studied by Femtosecond Transient Absorption, *J. Chem. Educ.*, 97 (12), 4482-4489 DOI: 10.1021/acs.jchemed.0c01056.
- 12. Rodriguez, J.-M. G., Harrison, A. R., and Becker N. M. (2020) Analyzing Students' Construction of Graphical Models: How Does Reaction Rate Change Over Time? *J. Chem. Educ.* 97 (11), 3948-3956 DOI: 10.1021/acs.jchemed.0c01036
- 13. Atkinson, M. B., Popova, M., Croissant, M., Reed, D. J., and Bretz, S. L. (2020) Development of the Reaction Coordinate Diagram Inventory: Measuring Student Thinking and Confidence *J. Chem. Educ.* 97 (7), 1841–1851 DOI: 10.1021/acs.jchemed.9b01186
- 14. McEvoy, J. P., and Kay, A. (2020) The Saturation Game: Teaching Protein—Ligand Binding with a Playing Card Analogy *J. Chem. Educ.* 97 (10), 3727–3730DOI: 10.1021/acs.jchemed.oco0837
- 15. Xian, J. and King, D. B. (2020) Teaching Kinetics and Equilibrium Topics Using Interlocking Building Bricks in Hands-on Activities *J. Chem. Educ.* 97 (2), 466-470 DOI: 10.1021/acs.jchemed.9b00515
- 16. Wallen, S. L., Dhau, J., Green, R., Wemple, L. B., Kelly, T., and Collins, B. (2020) Maker Chemistry: Exploring Redox Reactions in Introductory Laboratory through Light-Emitting Diode Printed Circuit Board Fabrication *J. Chem. Educ.* 97 (2), 490-496DOI: 10.1021/acs.jchemed.8b01061
- 17. Phillips, J. A., Jones, G. H., and Iski, E. V. (2019) Using a Guided-Inquiry Approach To Teach Michaelis—Menten Kinetics *J. Chem. Educ.* 96 (9), 1948–1954DOI: 10.1021/acs.jchemed.9b00031
- 18. Bennie, S.J., Ranaghan, K. E., Deeks, H., Goldsmith, H. E., O'Connor, M. B., Mulholland, A. J., and Glowacki, D. R. (2019) Teaching Enzyme Catalysis Using Interactive Molecular Dynamics in Virtual Reality *J. Chem. Educ.* 96 (11), 2488–2496 DOI: 10.1021/acs.jchemed.9b00181
- 19. Novak, I. (2020) Reversible Reactions: Extent of Reaction and Theoretical Yield *J. Chem. Educ.*, 97 (2), 443-447 DOI: 10.1021/acs.jchemed.9b0088
- 20. Nelson, K. A., and Bawendi, M. (2008) https://ocw.mit.edu/courses/chemistry/5-60-thermodynamics-kinetics-spring-2008/video-lectures.

L	Т	P	Cr
3	0	0	3

Course Title: Spectroscopic Analysis

Paper Code: CHM.524 Total Contact Hours: 45

Learning Outcome: At the end of this course student will be able to

- Identify various spectroscopic techniques (UV, IR, NMR and MS) used in organic synthesis for structure elucidation.
- Predict NMR spectra and various fragment-ions/peaks in MS of a given molecular structure.
- Analyze and interpret the combined spectroscopic data (UV-Vis, IR, ¹H & ¹³C NMR) for structural elucidation of unknown organic molecules.

Unit 1

11 Hours

UV-Visible spectroscopy: Introduction, role of solvents, chromophores and their interaction with UV-visible radiation. Woodward-Fieser rule for conjugated dienes and carbonyl compounds

Infrared Spectroscopy: Infrared radiation and its interaction with organic molecules, vibrational mode of bonds, effect of hydrogen bonding and conjugation on absorption bands, interpretation of IR spectra. FTIR.

Problem solving - Identification of the structure from the given UV and FTIR data

Unit 2

12 Hours

Nuclear magnetic resonance spectroscopy: Introduction, chemical shift and factors influencing chemical shift, reference standards and solvents. spin-spin coupling, coupling constants, long range coupling, effect of deuteration, integration of signals, interpretation of spectra, spin decoupling, double resonance and shift reagent methods, resonance of other nuclei e.g. ¹⁹F, ¹⁵N, ³¹P.

The role of external magnetic field on precessional frequency: Peer discussion

Unit 3

11 Hours

¹³C NMR: Introduction, Proton coupled and proton decoupled ¹³C NMR, nuclear overhauser enhancement (NOE), DEPT techniques, 2D NMR Correlation spectroscopy (COSY), Homo COSY (¹H-¹H COSY), Hetero COSY (¹H-¹³C COSY, HMQC), long range ¹H-¹³C COSY (HMBC), NOESY.

Problem solving - Identification of the structure from the given 1H and C-13 NMR data

Unit 4 11 Hours

Mass spectrometry: Basic principles and brief outline of instrumentation. Ion formation: EI, CI, FAB, MALDI, ESI, metastable ion, α -cleavage, McLafferty rearrangement, Retro-Diels-Alder cleavage, nitrogen rule, fragmentation process of organic molecules in relation to molecular structure determination. Relative abundance of isotopes, High resolution mass spectrometry (HRMS) and recent advances in mass spectrometry.

Problems for structure elucidation using the above spectroscopic techniques. Interpretation of various fragmentation peaks in the mass spectrum of the given sample

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Pavia, D. L., Lampman, G. M., Kriz, G. S., and Vyvyan, J. A. (2015). *Introduction to Spectroscopy*. Cengage Learning India Private Limited; 5th edition (14 January 2015).
- 2. Gross, J. H. (2017). *Mass Spectrometry: A Textbook*. Springer-Verlag Berlin Heidelberg.
- 3. Banwell, C. N., and McCash, E. M. (1994). *Fundamentals of Molecular Spectroscopy* (Vol. 851). New York: McGraw-Hill.
- 4. Dyer, J. R. (1965). Applications of Absorption Spectroscopy of Organic Compounds. Phi Learning.
- 5. Kalsi, P. S. (2007). *Spectroscopy of Organic Compounds*. New Age International.
- 6. Kemp, W. (2019, 2nd edition). *Organic Spectroscopy*, ELBS. MACMILLAN
- 7. Khopkar, S. M. (1998). Basic Concepts of Analytical Chemistry. New Age International.
- 8. Melinda, J.D. (2010). *Introduction to Solid NMR Spectroscopy*. Wiley India Pvt Ltd.
- 9. Silverstein, R. M., Webster, F. X., Kiemle, D. J., and Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley and sons.
- 10. Pretsch, E., Bühlmann, P., Badertscher, M. (2020). Structure Determination of Organic Compounds. Springer-Verlag Berlin Heidelberg
- 11. Webb, G. A. (2021). Annual Reports on NMR Spectroscopy. Elsevier

L	Т	P	Cr
3	0	0	3

Course Title: Molecular Spectroscopy

Paper Code: CHM.525 Total Contact Hours: 45

Learning Outcome: The students will be able to

- Apply microwave, infrared-vibration-rotation Raman and infra-red Spectroscopy for chemical analysis and prediction of molecular structure
- Demonstrate and apply electronic spectroscopy of different elements and simple molecules.
- Explore application of laser spectroscopy and photoelectron spectroscopy in materials and biomaterials.
- Demonstrate and elucidate the physical principles of nuclear magnetic and electron spin resonance spectroscopy.

Unit 1 11Hours Electronic Spectroscopy: Electronic transition, energy of electronic transition, selection rules, the Franck-Condon principle.

Microwave Spectroscopy: Basic principle and instrumentation, classification of molecules, selection rule in microwave spectroscopy, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities of spectral lines, non-rigid rotor, Stark effect, and applications of microwave spectroscopy.

Problem solving approach to determine the bond length of diatomic and polyatomic molecules and effect of isotopic substitution on transition frequencies.

Unit 2

12 Hours

Pure Vibrational Spectroscopy: Basic principle and instrumentation of IR spectroscopy, Review of harmonic oscillator, selection rules, vibrational energies of diatomic molecules, zero-point energy, force constant and bond strength, anharmonicity, vibration-rotation spectroscopy, Morse potential energy diagram, P, Q, R branches, vibrations of polyatomic molecules, overtones and hot bands. Applications of IR spectroscopy.

Raman Spectroscopy - Basic principle and instrumentation of Raman spectroscopy, classical and quantum theories of Raman Effect, vibrational-

rotational Raman spectra, selection rules, mutual exclusion principle, resonance Raman Spectroscopy, depolarization ratio, surface enhanced Raman spectroscopy, coherent anti-stokes Raman spectroscopy. Application of Raman spectroscopy.

Brainstorming on use of electronic, pure vibrational, pure rotational and vibrational-rotational spectroscopy in understanding chemical characteristics.

Unit 3

11 Hours

Magnetic Resonance Spectroscopy: Basic principles of NMR and ESR, instrumentation of NMR and ESR, magnetization vector and relaxation, NMR transitions, Bloch equation, relaxation effects and mechanism, effect of quadrupole nuclei, nuclear overhauser effect (NOE), multiple pulse methods, Hyperfine splitting in ESR. Application of NMR and ESR Spectroscopy. Understanding applications of magnetic resonance spectroscopy through peer learning and brainstorming.

Unit 4 Hours

Lasers and Laser Spectroscopy: Principles of laser action, pulsed lasers, examples of lasers: He-Ne, Nd-YAG, dye lasers.

Atomic Force Spectroscopy: Basic principle and instrumentation, application of single molecule force spectroscopy.

Photoelectron spectroscopy: Basic principle and instrumentation, photoelectric effect, UV photoelectron spectroscopy UPS, X-ray photoelectron spectroscopy XPS. Application of XPS and UPS.

Understanding application and instrumentation of laser, photoelectron and atomic force spectroscopy through peer discussion.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming.

- 1. Hollas, J. M. (2004). *Modern Spectroscopy*. John Wiley and Sons.
- 2. Lakowicz, J. R. (2006). *Principles of Fluorescence Spectroscopy*. Springer.
- 3. Barrow, G. M. (2007) *Physical Chemistry*. Tata McGraw-Hill Publishers.
- 4. Banwell, C. N., and McCash, E. M. (1994). Fundamentals of Molecular Spectroscopy (Vol. 851). New York: McGraw-Hill.
- 5. Carrington, A., and McLachlan, A. D. (1967). Introduction to Magnetic Resonance: With Applications to Chemistry and Chemical Physics. Chapman and Hall, London.

- 6. Lynden-Bell, R. M., and Harris, R. K. (1969). *Nuclear Magnetic Resonance Spectroscopy*. Appleton–Century–Crofts.
- 7. Reilley, C. N., Everhart, D. S., and Ho, F. F. L. (1982). *Applied Electron Spectroscopy for Chemical Analysis. Chemical Analysis*, 63, 105. John Wiley.
- 8. Chang, R. (1971). Basic Principles of Spectroscopy. McGraw-Hill.
- 9. Ghosh, P. K. (1983). *Introduction to Photoelectron Spectroscopy*. John Wileyand Sons, New York.
- 10. Günther, H. (2013). NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry. John Wiley and Sons.
- 11. Atkins' P. (2014) Physical Chemistry, Peter Atkins and Julio Paula, Oxford University Press; 10th Ed.
- 12. Banwell, C. N. (2013). Fundamentals of Molecular Spectroscopy. Tata McGraw-Hill Education IV edition.
- 13. Rita Kakkar, R. (2015) Atomic and Molecule Spectroscopy: Basic Concepts and Applications, Cambridge University Press, 2015.
- 14. J L McHale (2008) Molecular Spectroscopy, Pearson Education India

L	Т	P	Cr
0	0	4	2

Course Title: Practical Physical Chemistry

Paper Code: CHM.527 Total Contact Hours: 60

Learning Outcome: The students will able to

- Develop skills on titrimetric analysis using conductivity meter, potentiometer and pH meter as well as buffer preparation and use.
- Hands on skills in viscometer, refractometer and spectrophotometer for different applications.
 - 1. Determination of behavior and strength of a given acid/base by titrating with a base/acid conductometrically.
 - 2. Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO₄, BaSO₄) conductometrically.
 - 3. Determination standard electrode potential of Fe²⁺/Fe³⁺ system by potentiometer using (A) Potassium Permanganate (B) Ceric ammonium nitrate solution.
 - 4. Preparation of buffers and measurement of their pH and determination of stability constant for Cu(II)-glycinate complex using potentiometry.
 - 5. Determination of pK_a of acetic acid and H₃PO₄ by potentiometric titration using NaOH.
 - 6. Determination of (A) relative and absolute viscosity (B) Surface tension of a given liquid.

- 7. Determination of refractive indices (RI) of given liquids and determination of the concentration from RI.
- 8. Verification of the Lambert-Beer's law and determination of stability constant of Fe(III)-salicylic acid complex by spectrophotometer.
- 9. To verify Freundlich and Langmuir adsorption isotherms for adsorption of acetic acid on activated charcoal.
- 10. Determination of partition coefficient of (A) benzoic acid between organic solvent and water. (B) iodine between water and octanol and determination of equilibrium constant of tri-iodide.
- 11. Determination of (A) rate constant and energy of activation of hydrolysis of an ester and (B) study the effect of ionic strength on reaction rate.
- 12. Determination of (A) order and energy of activation and (B) effect of variation of ionic strength on the rate of $S_2O_8^{2-} + I^- + S_0^{2-} + I_2$.
- 13. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine-clock reaction.

Mode of Transactions: Demonstration, Experimentation, handing instruments, Explanation of data

Activity Based Learning:

- 1. Demonstration and application of potentiometry, conductometry, spectrophotometry, viscometer and stalagmometer.
- 2. Team activity of practical and observation recording for kinetic and thermodynamic parameters for chemical reactions.

- 1. Nad, A. K., Mahapatra, B. and Ghoshal, A. (2014). *An Advanced Course in Practical Chemistry*. New Central Book Agency (P) Ltd.
- 2. Maity, S., and Ghosh, N. (2012). *Physical Chemistry Practical*. New Central Book Agency (P) Ltd.
- 3. Elias, A. J. (2002). A Collection of Interesting General Chemistry Experiments. Universities Press.
- 4. Khosla, B.D., Garg, V.C., and Gulati A.R. (2007). Senior Practical Physical Chemistry. S. Chandand Sons.
- 5. Yadav, J. B. (2006). *Advanced Practical Physical Chemistry*. Krishna Prakashan Media.
- 6. Das, R. C., and Behera, B. (1983). *Experimental Physical Chemistry*. Tata McGraw-Hill.
- 7. James, A. M., and Prichard, F. E. (1974). *Practical Physical Chemistry*. New York: Longman.
- 8. Ghosh, J.C. (1990). Experiments in Physical Chemistry, Bharati Bhavan.

L	Т	P	Cr
0	0	4	2

Course Title: Computational and Structural Chemistry (Practical)

Paper Code: CHM.529 Total Contact Hours: 60

Learning Outcomes: After completing this course, the learner will be:

- 1. Skilled in various chemistry software needed for higher studies.
- 2. Develop knowledge skills and understanding of structure elucidation of unknown compounds via spectral interpretation of ¹H, ¹³C NMR, IR, UV and Mass spectrum.
- 3. Select and apply the data analytics to every process and analysis in chemistry, thereby bringing in quality control to his work in hand.

ChemDraw, Chem-Sketch, Draw the structure of simple aliphatic, aromatic, heterocyclic organic compounds with substituents. Get the correct IUPAC name and prediction of ¹HNMR signals.

Exposure to Softwares required for processing of raw FID NMR files, Molecular docking using Schrodinger/MOE Softwares and DFT studies using Gaussian software.

Single crystal structure solving of various compounds and complexes using X-Ray Diffraction (XRD) software Olex-2.

Spectral interpretation: (1H, 13C NMR, IR, UV and Mass spectrum)

Interpretation of UV, IR, NMR (1D & 2D NMR) and mass spectrum

Structural elucidation of some unknown compounds based on the provided 1H, 13C NMR, IR, UV and Mass spectrum of a given compound.

- 1. Determination of Detection limit, Quantitation limit and for instrumental method and method of analysis.
- 2. Determination of quality control parameters for a method of analysis.
- 3. Determination of Mean. Mode and Median, Skewness and Kurtosis, FWHM for chromatographic data.
- 4. Linear least square fitting for calibration of spectrometer
- 5. Non-Linear least square fitting for adsorption and kinetic data.
- 6. Determination of ANOVA for intralaboratory testing.
- 7. Error function and residual analysis of Linear and Non-linear least square fitting
- 8. Optimization of process and analysis using Factor analysis, Principle Component Analysis

- 9. Optimization of process using response surface methodology
- 10. Determination of charges, pKa and electrostatic free energy of enzymes and proteins using pKa calculation software.

Suggested Readings

- 1. Pavia, D. L., Lampman, G. M., Kriz, G. S., and Vyvyan, J. A. (2015). *Introduction to Spectroscopy*. Cengage Learning India Private Limited; 5th edition.
- 2. Gross, J. H. (2017). *Mass Spectrometry: A Textbook*. Springer-Verlag Berlin Heidelberg.
- 3. Pasto, D.P., Johnson, C., Miller, M. (2010). Experiments and Techniques in Organic Chemistry, Prentice Hall.
- 4. Vogel, A.I. (2003). Text Book of Practical Organic Chemistry, Pearson
- 5. Armarego, W. L., & Chai, C. (2012). Purification of Laboratory Chemicals. Butterworth-Heinemann.
- 6. Findeisen, M., (2013). 50 And More Essential NMR Experiments: A Detailed Guide. John Willey & Sons.
- 7. Fine, J. A., Rajasekar, A. A., Jethava, K. P., & Chopra, G. (2020). Spectral deep learning for prediction and prospective validation of functional groups. *Chemical Science*, 11(18), 4618–4630.
- 8. Yorck, M.M., and Neuhold, M., (2007) Practical Data Analysis in Chemistry, 26, Elsevier Science.
- 9. https://www.practicaldatascience.org/html/pandas_series.html.
- 10. Leszczynski, J., Shukla, M. (2012) Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends, Springer Netherlands.

L	Т	P	C
			r
1	0	0	1

Course Title: Entrepreneurship

Paper Code: CHM.530

Total Hours: 15

Learning Outcomes: On the completion of this course, students will be able

- a. To develop understanding about problems and prospects in entrepreneurship.
- b. To gain insights about entrepreneurial behaviour and skills.
- c. To develop understanding about writing business plan/project proposals & managing start-up issues.

UNIT I Hours

Entrepreneurial Structure; Nature, Characteristics, functions and its role in economic development, Entrepreneurship - problems and prospects in India Entrepreneurial Behaviour and Skills

Role of Entrepreneurship in economic development of India through peer group discussion.

UNIT II Hours

Role of industries/entrepreneur's associations and self-help groups, Funding opportunities for start-ups. Basic start-up problems, Preliminary contracts with the vendors, suppliers, bankers, principal customers. Contents of business plan/ project proposal

Peer discussion on various start-ups and recent funding opportunities.

UNIT III
Hours

Intellectual property: Concept of intellectual property, Industrial property: Patents, Trademarks, GI, copyrights and related rights. WTO, WIPO and various treaties: Trade related aspects of intellectual property rights (TRIPS), Trade related investment measures (TRIMS). Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

Case studies on traditional knowledge and patent issues; Turmeric, Basmati and neem cases

UNIT IV
Hours

Key business concepts

Business plans, market need, project management and routes to market. Chemistry in Industry, Current challenges and opportunities, role of chemistry in India and global economies.

Use of hazardous chemicals in Industries and the Importance of development of cost-effective and green technology.

Group presentations on the Importance of development of cost-effective and benign technologies

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

References:

- 1. Nwaeke, L.I. (2002), Business Concepts and Perspectives, Springfield Publishers.
- 2. Silva, T. D. (2013), Essential Management Skills for Pharmacy and Business Managers, CRC Press.
- 3. Pandey, N.; Dhami, K. (2014), Intellectual Property Rights, PHI Learning Pvt. Ltd.
- 4. Acharya, N.K. (2001), Text Book of Intellectual Property Rights, Asia Law House.
- 5. Ganguli, P. (2001), Intellectual Property Rights: unleashing the knowledge economy. Tata McGraw Hill.
- 6. Nithyananda K.V. (2019), Intellectual Property Rights, Protection and Management. Cengage Learning India Pvt. Ltd.
- 7. de Jong, A., De Ruyter, K., Keeling, D. I., Polyakova, A., & Ringberg, T. (2021). Key trends in business-to-business services marketing strategies: Developing a practice-based research agenda. Industrial Marketing Management, 93, 1-9.

L	Т	P	Cr
0	0	4	2

Course Title: Advanced Applied Practical Chemistry

Paper Code: CAC.551 Total Contact Hours: 60

Learning Outcome: At the end of this course students will be able to

- Identify various agents used for drying of solvents and their disposal.
- Separate and purify the desired product from an organic reaction.
- Characterize organic compounds using various spectroscopic techniques.
- Realize the impact of various coupling and click chemistry strategies for construction of value added chemicals.
- Biochemical, biophysical and structural characterizations of biomacromolecules.

Experiments:

Solvent Drying: Use of sodium metal for drying of toluene and precautions while quenching the residual sodium. Drying of DCM using P_2O_5 and safe disposal of residual P_2O_5 .

1. **Synthesis**: Separation and purification of organic compounds by column chromatography, percentage yield calculation (any Five)

Preparation of allylic alcohols *via* Baylis-Hillman reaction using DABCO as a catalyst and their characterization through various spectroscopic techniques.

To study the reaction of vanillin with malonic acid for the synthesis of 4- Vinylguaiacol.

To study Buchwald-Hartwig reaction of aryl halide with an amine using Cu-based catalyst.

Synthesis of triazole *via* reaction of phenylacetylene with azide (Huisgen cycloaddition).

Synthesis of stilbenes *via* Heck coupling Strategy.

To study decarboxylation of Ferulic acid under microwave irradiation. To study dehydration of benzylic alcohols using imidazolium based ionic liquid.

To synthesize benzofused heterocyclic compounds (any one)

(i) Coumarin (ii) benzothiazole

To synthesize 2-phenyl-1,3,4-oxadiazole from benzhydrazide.

To synthesize substituted benzodiazepine from chalcone *via* reflux conditions.

To study synthesis of Dilantin *via* benzylic-acid rearrangement To study the rearrangement of benzopinacol into benzopinacolone To study the three component coupling for the synthesis of (any one)

- o dihydropyrimidinone (via Biginelli reaction)
- o propargylamine (via A³-coupling)
- 2. Determination of concentrations of proteins and DNA using spectrophotometer
- 3. Structural analysis of amino acids and proteins using CD, NMR and Fluorescence spectrometer.
- 4. Study of thermal denaturation (T_m and DH_m) of proteins and DNA using UV-Visible spectrophotometer, CD spectrometer and DSC.
- 5. Measurement of zeta potential and sizes of nanoparticles by DLS
- 6. Determination of Michaelis-Menten (Km) constant in enzyme kinetics.
- 7. Particle size and hydrodynamic radii analysis for adsorbents, protein or nanoparticles
- 8. Measurement of affinity constant of metal complex or metal binding to protein by ITC

Mode of Transactions: Demonstration, PPT, videos, Lecture cum demonstration

Suggested Readings

1. Vogel, A.I. (2003) Textbook of Practical Organic Chemistry. ELBS, Longman Group Ltd.

- 2. Mann, F.G. and Saunders, B.C. (2009) *Practical Organic Chemistry*. Orient Longman Pvt. Ltd.
- 3. Leonard, J. and Lygo, B. (1995) Advanced Practical Organic Chemistry. Chapman and Hall.
- 4. Armarego, W.L. and Chai, C. (2012) *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
- 5. Kaur, P. Kumar B. Gurjar, K.K. Kumar, R, Kumar, V, and Kumar, R. (2021) Metal-and solvent-free multicomponent decarboxylative A3-coupling for the synthesis of propargylamines: Experimental, computational and biological investigations, *The Journal of Organic Chemistry*, 2020, 85(4), 2231-2241
- 6. Young, J.A. (1991) Improving Safety in the Chemical Laboratory: A Practical Guide. Wiley Publishing.
- 7. Cantor, C.R. and Schimmel, P.R (1980). Biophysical Chemistry Part II: Techniques for the Study of Biological Structure and Function, W. H. Freeman & Co., New York
- 8. Van Hlde, K.E., Johnson W.C. and Ho John, P.S. (2005) Principles of Physical Biochemistry" 2 nd edition, Pearson Prentice Hall.
- 9. Wilson, J. M., Newcombe, R. J., and Denaro, A. R., (2016) Experiments in Physical Chemistry, 2nd Ed., Elsevier Science
- 10. Haghi, A. K., Aguilar, C. N., Cortes, J. S. and Ascacio-Valdés, J. A. (2021) Practical Applications of Physical Chemistry in Food Science and Technology, Apple Academic Press.
- 11. Kumari, A., Anand, R., Kumari, R. (2019) Physical Chemistry Laboratory Manual: An Interdisciplinary Approach, I K International Publishing House Pvt. Limited.
- 12. Firth, J. B. (2018) Practical Physical Chemistry, Creative Media Partners, LLC.

L	Т	P	Cr
3	0	0	3

Course Tile: Pharmaceutical Products

Paper Code: CAC.585 Credits Hours: 45

Learning Outcome: The students will be able to

- Describe the medicinal importance of various herbal products.
- Identify various commercial processes relevant in oleo chemical industry.

• Explore fats and oil as raw material for the synthesis of value added chemicals.

Unit 1 12 Hours

Herbal Products:

General Properties, Chemistry, Phytoconstituents and bioactive constituents and medicinal importance

Alkaloids Containing Herbal Drugs: Papaver somniferum (morphine), Rauvolfia serpentina (reserpine), Atropa belladonna (atropine), Ephedra gerardiana (ephedrine), biosynthesis of alkaloids.

Terpenes Containing Herbal Drugs: Lemon grass oil (citral and geraniol), Artemisia annua (artemisinin) and Taxus baccata, biosynthesis of terpenoids **Phenolics containing Herbal Drugs**: Vitis vinifera (resveratrol), Pterocarpus marsupium (Pterostilbene)

Various Berry fruits (strawberry, cherry, raspberry etc.).

Structures and biological activity of alkaloids and terpenoids through group presentations

Group project on recent advances on natural product based drug development

Unit 2

Hours

Edible Oils and Fats: General study of the quality assessment, hydrogenation of oils, rancidity, iodine value, acid value, saponification value, Reichert-Meissel value, Polenski value and Kirschner value, adulteration of oils and fats, modifications to produce specialty fats (structured fats, nutraceuticals). Essential fatty acids: ω -3 and ω -6 fatty acids.

Group project on preparation of various oils and fats and check their chemical composition.

Unit 3 11 Hours

Soap: Introduction, manufacturing process different types of soap and their composition, Recovery of glycerin from soap spent lye. Metathesis and co metathesis reactions of fats and oils and their application in oleo chemical industry. hydroformylation reaction, cracking of fatty acids and fatty acid esters.

Group presentation on manufacturing process of different types of soap

Unit 4

Hours

Cosmetics and Perfumes: Cosmetic necessities: Protective and antimicrobials, Astringents; safety issues of cosmetics. Storage and preparation of herbal drugs for commercial market. Essential oils and their importance in cosmetic industries.

Antiperspirants, artificial and natural flavours, colours and preservatives, artificial sweeteners.

Peer learning on the recent research related to the impact of various preservatives and sugar substitutes on human health

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Gunstone, F., (2004). *The Chemistry of Oils and Fats.* Blackwell Publishing Ltd, UK.
- 2. Rahman, A. U. (Ed.). (2006). Studies in Natural Products Chemistry (Vol. 33). Elsevier.
- 3. Jain, P.C. and Jain M. (2007). *Engineering Chemistry*. Dhanpat Rai and Sons.
- 4. Sharma, B. K. (1991). Industrial Chemistry. Krishna Prakashan Media.
- 5. Patrick, G. L. (2013). *An Introduction to Medicinal Chemistry*. Oxford university press.
- 6. Singh, H., and Kapoor, V.K., (2007). *Medicinal and Pharmaceutical Chemistry*. VallabhPrakashan, Pitampura, New Delhi.
- 7. Foye, W. O. (2008). Foye's Principles of Medicinal Chemistry. Lippincott Williams and Wilkins.
- 8. Poucher, W. A. (2012). *Poucher's Perfumes, Cosmetics and Soaps: Volume* 3: *Cosmetics.* Springer Science and Business Media.
- 9. Edwards, S. E., da Costa Rocha, I., Heinrich, M., and Williamson, E. M. (2015). *Phytopharmacy: An Evidence-Based Guide to Herbal Medicinal Products*. John Wiley and Sons.
- Daley. S. K., Cordell, G. A., Biologically Significant and Recently Isolated Alkaloids from Endophytic Fungi, *J. Nat. Prod.* 2021, 84, 3, 871–897.

11. Thomas, W. P., Pronin, S. V., New Methods and Strategies in the Synthesis of Terpenoid Natural Products, *Acc. Chem. Res.* 2021, 54, 6, 1347–1359.

L	Т	P	Cr
3	0	0	3

Course Title: Quality Control in Laboratory and Manufacturing

Code: CAC.553
Total Lectures: 45

Learning Outcome: The students will be able to

- Demonstrate and apply the various statistical tools for the quality control of the analytical results and its implications to regulatory approvals.
- Elucidate the good laboratory and manufacturing practices.

Unit I 11 Hours

Statistical. Method of Least squares and weighted least squares formalism. Use of certified reference materials and procedures for interlaboratory comparisons. Definition of limits of detection and sensitivity, and concept of standard addition to assess matrix effects. Uncertainty Calculations.

Statistical quality control would be understood through problem solving activity.

Unit II Hours

Concept of Total Quality Management, philosophy of Good Manufacturing Practice (GMP), ISO 9000 and ISO 14798 (NABL Accreditation). Organization and personnel, responsibilities, training, hygiene, personnel records.

Premises: Location, design, plan layout, construction, maintenance of sterile areas, control of contamination. Equipment, selection purchase specifications, preventive maintenance of equipment, cleaning of equipment.

Requirements of quality control in pharmaceutical manufacturing would be learnt through field visit.

Unit III 11 Hours

Quality control laboratory, Good Laboratory Practice(GLP), responsibilities of management, Study Director, Quality Assurance Unit, and Individual,

routine controls, instruments, reagents, sampling plans, standard test procedures, protocols, non-clinical testing, controls on animal house, data generation and storage, quality control documentation, retention samples, records. Complaints and recalls, evaluation of complaints, recall procedures, related records and documents.

Good laboratory practices would be understood with card game and peer learning.

Unit IV 11 Hours

Regulatory aspects of pharmaceutical and bulk drug manufacture. DRA, FDA, CPMP, ICH guidelines. Regulatory Aspects of Environmental and Food Testing USEPA, MoEF, MoFPI, AOAC guidelines. Validation: Qualification (IQ/PQ/OQ), validation and calibration of equipment's, Evaluation of Analytical data. Drug approval process, patent application and WHO certification.

Regulatory requirements of various international and national governing bodies on quality laboratory and manufacturing would be understood through peer learning.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

- 1. Miller, J. C., and Miller, J. N. (2010). *Statistics for Analytical Chemistry*. Pearson Education Ltd.
- 2. http://www.who.int/water_sanitation_health/resourcesquality/wqmchap9.pdf
- 3. https://www.unece.org/fileadmin/DAM/env/water/publications/documents/guidancelaboratories.pdf.
- 4. EURACHEM / CITAC (2012) Quantifying Uncertainty in Analytical Measurement, EURACHEM / CITAC Guide CG 4, 3rd Edition, https://www.eurachem.org/images/stories/Guides/pdf/QUAM2012_P1.pdf .
- 5. Westgard, J. O., Barry, P. L. (2016) Basic QC Practices: Training in Statistical Quality Control for Medical Laboratories, 4th ed., Westgard Quality Corporation.
- 6. Kenkel, J. (2014) Analytical Chemistry for Technicians, 4th ed., CRC Press.
- 7. Konieczka, P., Namiesnik, J., (2018) Quality Assurance and Quality Control in the Analytical Chemical Laboratory: A Practical Approach, 2nd ed. CRC Press.
- 8. WHO (2011) Laboratory Quality Management System Handbook.

- 9. Zaman, G., (2018) Quality Control in Laboratory, Intech Open Publishing.
- 10. Hasnain, M.S., Beg, S., (2019) Pharmaceutical Quality by Design: Principles and Applications, Elsevier Science.
- 11. Welty G., (2013) Quality Assurance: Problem Solving and Training Strategies for Success in the Pharmaceutical and Life Science Industries Woodhead Publishing.
- 12. Haider, S. I., Asif, S. E., (2016) Quality Control Training Manual: Comprehensive Training Guide for API, Finished Pharmaceutical and Biotechnologies Laboratories, CRC Press.
- 13. Gibson, M., Schlindwein, W. S. (2018) Pharmaceutical Quality by Design: A Practical Approach, Wiley Publishing.
- 14. Gad, S. C. (2008) Pharmaceutical Manufacturing Handbook: Regulations and Quality, Wiley Publishing.
- 15. Luthra, S., Garg, D., Agarwal, A., Mangla, S. K. (2020) Total Quality Management (TQM): Principles, Methods, and Applications, CRC Press.
- 16. Montgomery, D. C., (2020) Introduction to Statistical Quality Control, Wiley Publishing.
- 17. Bunn, G. P. (2019) Good Manufacturing Practices for Pharmaceuticals, 7th Edition, CRC Press
- 18. Shewhart, W. A. (2012) Statistical Method from the Viewpoint of Quality Control, Dover Publication.

Course Title: Advanced Logics in Chemistry	L	Т	P	Cr
Paper Code: CHM.559	2	0	0	2

Total Contact Hours: 30

Learning Outcome: This course is designed to exercise various problems in organic synthesis so that students can compete for national level competitive examinations such as UGC-CSIR-NET, GATE etc. After completion of this course student will be able to

- Interpret spectroscopic data and solve various problems of structure elucidation.
- Identify the product of various pericyclic reactions including stereoselective aspects of various organic transformations.
- Compare the reactivity of various heterocyclic compounds and utility of natural products.

- Know the aspects of structural and bonding of ionic, covalent and coordination molecules and compounds.
- Elucidate the aspects of s, p, d and f-block elements
- Physical concept involving in quantities errors, Kinetics. Thermodynamics, photochemistry and electrochemistry.

Unit 1 Thours

Combined Structure problems: Exercises of structure elucidation of unknown compounds *via* combined spectral interpretation of IR, UV-vis, ¹H and ¹³C NMR and mass spectra, along with two-dimensional NMR spectroscopy. IUPAC nomenclature of organic molecules including regioand stereoisomers.

Organic reaction mechanisms: involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways. Various strategies for asymmetric synthesis and its applications in natural products and drug molecules.

Problem solving for the identification of the structure of molecules based on given NMR, UV, IR and Mass data. Peer group discussion on naming organic reactions and their mechanisms.

Unit 2 Hours

Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents: organic, inorganic, organometallic and enzymatic. stereoselective transformations. Green catalysts in organic synthesis. Exercises on stereochemical aspects of various pericyclic reactions.

Reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S) and their utility in organic synthesis. Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, terpenes and alkaloids.

Deliberation on various reagents, photochemical and pericyclic reactions and their mechanisms. Debate on selective reducing and oxidizing reagents in organic synthesis. Peer group discussion on biosynthesis of heterocycles and natural products.

Structure and bonding: Electronic configuration of atoms (L–S coupling) and the periodic properties of elements; Ionic radii, Ionization potential, electron affinity, electronegativity; concept of hybridization. Molecular orbitals and electronic configuration of homo– and hetero–nuclear diatomic molecules. Shape of polyatomic molecules; VSEPR theory, Symmetry elements and point groups for simple molecules. Acid and bases concepts, pH and pK_a, HSAB concept, Buffer solution. Properties of solid state and solution phase, reaction mechanism in metal compounds, cluster chemistry, Inorganic spectroscopy.

Aspects of s, p, d and f-block elements: General characteristics of each block. Chemistry of representative (s and p-block) elements, Coordination chemistry of transition elements. Chemistry of lanthanide and Actinides.

debate and problem solving of various concepts involved in group theory, mechanism, transition and inner transition metals, p-block clusters, ESR and Mossbauer spectroscopy.

Unit 4 8 Hours

Thermodynamics: Concepts involved in first, second and third law of thermodynamic, Maxwell relations, Helmholtz and Gibbs Energies, equilibrium constant, temperature-dependence of equilibrium constant and Van't Hoff equation, Colligative properties of solutions.

Electrochemistry: Ionic equilibria, ion conduction mechanism, solutions of nonelectrolytes and electrolytes, electrolytic conductance –Kohlrausch's Law, transport number and its determination, Nernst equation, redox systems, electrochemical cells.

Basics of Photochemistry: Absorption, excitation, laws of photochemistry, quantum yield, lifetime of excited states, photochemical stages-primary and secondary process.

Kinetics: Introduction, rates of chemical reactions, Kinetics of photochemical reactions.

Learning through peer discussion different physical concepts involved in chemical kinetics, thermodynamics, photochemistry and electrochemistry.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Pavia, D. L., Lampman, G. M., Kriz, G. S., and Vyavan, J. R., (2010). *Introduction to Spectroscopy*. Harcourt College, NY.
- 2. Dewick, P. M., (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Wiley and Sons, UK.
- 3. Finar, I. L. (2006). Organic Chemistry: Stereochemistry and the Chemistry of Natural Products. Dorling Kindersley Pvt. Ltd., India.
- 4. Claydon, J., Greeves, N., Warren, S. and Wother, P., (2001). Organic Chemistry. Oxford University Press, UK.
- 5. Fleming, I., (2015). Pericyclic Reactions. Oxford University Press.
- 6. Carey B. F. A., and Sundberg R. J., (2007). *Advanced Organic Chemistry Part B.* Springer Science and Business Media Ltd.
- 7. Yadav, L. D. S., Singh, J., and Singh, J. (2017). Organic Synthesis, Pragati Prakashan, India.
- 8. Norman, R. O. C., and Coxon, J. M. (1993). Principle of Organic Synthesis, CRC Press.
- 9. Cotton, F. A., and Wilkinson, G. (1988). Advanced Inorganic Chemistry (Vol. 545). New York: Wiley.
- 10. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). Inorganic Chemistry: Principles of Structure and Reactivity. Pearson Education India.
- 11. Greenwood, N. N., and Earnshaw, A. (2012). Chemistry of the Elements. Elsevier.
- 12. Miessler, G. L. and Tarr, D. A. (2011) Inorganic Chemistry, Pearson Education.
- 13. Atkins, P. (2010). Shriver and Atkins' Inorganic Chemistry. Oxford University Press, USA.
- 14. Barrow, G. M. (2007) Physical Chemistry. Tata McGraw-Hill Publishers. 7. Kapoor, K. L. (2011) Text Book of Physical Chemistry. 3/5, Macmillan Publishers.
- 15. Atkins, P. and De Paula, J. (2009) Atkins' Physical Chemistry. Oxford University Press.
- 16. Moore, J. W. and Pearson, R. G. (1981) Kinetics and Mechanism. John Wiley and Sons.
- 17. Puri, B. R., Sharma L.R. and Pathania, M. S. (2013) Principles of Physical Chemistry. Vishal Publishing Company.
- 18. Laidler, K. J. (1987). Chemical Kinetics. Pearson Education Ltd. 50
- 19. Rohatgi-Mukherjee, K. K., (1986). Fundamentals of Photochemistry. New Age International.
- 20. Stein, T. H., Vasiliu, M., Arduengo, A. J. Lewis Acidity and Basicity: Another Measure of Carbene Reactivity, *J. Phys. Chem. A* 2020, 124, 29, 6096–6103.
- 21. Gulevich, A. V., Dudnik, A. S., Chernyak, N., and Gevorgyan, V., Transition Metal–Mediated Synthesis of Monocyclic Aromatic Heterocycles. Chemical Reviews 2013, 113, 3084–3213.

L	Т	P	Cr
3	0	0	3

Course Title: Inorganic Chemistry-III

Paper Code: CHM.551 Total Contact Hours: 45

Learning Outcome: The students will be able to

Details on f-block elements properties

- Structural support to inorganic compounds through spectroscopic techniques
- Understanding the nuclear behaviour of various nucleoids.

Unit 1

10 Hours

Lanthanides, actinides and super-heavy elements: Coordination chemistry, magnetic and spectral properties, comparison of general properties of lanthanides and actinides, comparison with d-block elements, organolanthanides and actinides, analytical application of lanthanides and actinides-lanthanides as shift reagents and high temperature super conductors.

Group discussion on comparative properties and problem solving of lanthanide and Actinide elements.

Unit2

Hours

Nuclear Magnetic Resonance (NMR) and Electron Spin Resonance (ESR) Spectroscopy:

NMR: Basic concepts of NMR with emphasis on ³¹P, ¹⁹F, ²⁹Si, ¹¹B, ¹⁰B, ⁵⁷Se, ¹²⁵Te, ⁹⁵Mo, ¹⁰⁹Ag, ¹⁹⁵Pt, ¹¹⁹ Sn and explanation with appropriate examples. NMR study in Fluxional organometallic compounds.

ESR: Basic elements of ESR, Fine structure of ESR Signals transition metal ions, Zero-field Splitting, Kramer's Degeneracy, Hyperfine Splitting of various free radical spin polarization for atoms and transition metal ions, spin orbit coupling and significance of g-tensors, application of transition metal complexes (having one unpaired electron) including biological systems.

Hand on experience of inorganic complexes for resonance spectroscopy using NMR instrument and structural elucidation.

Unit3 10 Hours

Mossbauer Spectroscopy: Basic principles, spectral parameters and spectrum display, application of the technique to the studies of (1) bonding and structures of Fe²⁺ and Fe³⁺ compounds including those of intermediate spin, (2) Sn²⁺ and Sn⁴⁺ compounds – nature of M–L bond, coordination number, structure and (3) detection of oxidation state and non-equivalent MB atoms.

Peer discussion on basic parameters and technique implication for structural elucidation of iron and tin contain compounds using Mossbauer Spectroscopy

Unit4

Hours

Nuclear Chemistry: Classification of nuclides, nuclear stability, atomic energy, types of nuclear reactions-fission and fusion, nuclear decay laws, radioanalytical techniques.

Brainstorming discussion of nuclear reaction and atomic energy.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

- 1. Cotton, F.A. and Lippard, S.J., (1998). *Progress in Inorganic Chemistry*. Vol. 8, Wiley Internationals.
- 2. Lever, A.B.P., (1984). *Inorganic Electronic Spectroscopy*. Elsevier Science Publishers B.V.
- 3. Parish, R.V., (1990). NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry. Ellis Harwood.
- 4. Silverstein, R.M., Bassler, G.C., and Morrill, T.C. (2002). *Spectrometric Identification of Organic Compounds*. John Wiley and Sons.
- 5. Abraham, R. J., Fisher, J., and Loftus, P. (1988). *Introduction to NMR spectroscopy*. Wiley.
- 6. Martin, M. L., Delpuech, J. J., and Martin, G. J. J. (1980). *Practical NMR spectroscopy*. Heyden.
- 7. Williams, D. H., and Fleming, I. (1980). Spectroscopic Methods in Organic Chemistry. McGraw-Hill.
- 8. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
- 9. Lee, J. D. Concise Inorganic Chemistry: Fifth Edition (2012). Elsevier.
- 10. Kent, B. Inorganic Chemistry: Reactions, Structures and Mechanisms (12 June 2019), NY Research Press.
- 11. Close, D. Principles of Inorganic Chemistry (19 June 2019), Larsen and Keller Education

L	Т	P	Cr
3	0	0	3

Course Title: Organic Chemistry-III

Paper Code: CHM.552 Total Contact Hours: 45

Learning Outcome: The students will be able to

- Identify various retrosynthetic strategies and design the synthesis of target molecules.
- Explore various oxidizing and reducing reagents in a logical manner for their application in functional group transformation in organic synthesis.
- Compare the reactivity of smaller, five and six membered heterocyclic compounds and perform their synthesis.

Unit 1 11 Hours

Retrosynthesis: Synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination, criteria for selection of target, linear and convergent synthesis, retrosynthetic analysis involving chemoselectivity, reversal of polarity (umpolung), importance of the order of events in organic synthesis. One group and two group C-X disconnections, two group C-C disconnections; Diels-Alder reaction, control in carbonyl condensation.

Brainstorming on identification of the retrosynthetic route of some recently FDA approved commercial drug molecules.

Learning through peer discussion on order of events in organic synthesis.

Unit 2 Hours

Metal and non-metal mediated oxidation: Mechanism, selectivity, stereochemistry and applications of oxidation reactions, Baeyer-Villiger, Oppenauer oxidation, oxidation reactions using DDQ, NBS, Pb(OAc)₄, Selenium dioxide, PCC, PDC, Cr and Mn based reagents, phase transfer catalysis, Periodic acid, Ceric ammonium nitrate, OsO₄, Swern oxidation, hydroboration, Sharpless asymmetric epoxidation, epoxidations using peracids. Recent approaches for oxidation using green oxidants.

Demonstration on the synthesis and application of oxidizing agents like PCC. Peer discussion on green oxidizing agents.

Unit 3 Hours **Metal mediated reduction:** Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts (Lindlar, Rosenmund, Adam's catalysts), Wilkinson's catalyst, Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Pondorff-Verley reduction, dissolving metal reductions, Birch reduction, Reductions using metal hydride NaBH₄, Luche reduction, NaBH₃CN, L-selectride, K-selectride, NaBH(OAc)₃, LiAlH₄, DIBAL.

Peer discussion on selective use and careful handling of reducing agents.

Unit 4 Hours

Heterocyclic Chemistry: Systematic (Hantzsch-Widman system) and replacement nomenclature for monocyclic, fused and bridged heterocycles, aromatic heterocycle, non-aromatic heterocycle: bond angle and torsional strains and their consequences in small ring heterocycles, conformation of six-membered heterocycles.

Three-membered and four-membered heterocycles: aziridines, oxiranes, thiranes, azetidines, oxetanes.

Five membered heterocycles containing two heteroatoms (S, N, O): Diazoles (imidazole, pyrazole), triazoles, oxazoles and thiazoles.

Benzo-fused five-membered heterocycles: Indoles, benzofurans and benzimidazoles.

Six-membered heterocycles: Synthesis and reactions of coumarins, chromones.

Debate on reactivity order, basic and aromatic character of five- and six-membered heterocycles containing one and two heteroatoms.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Warren, S., (2010). Organic synthesis: The Synthon Approach. John Wileyand Sons.
- 2. Warren, S., and Wyatt, P., (2010). *Designing Organic Synthesis: A Disconnection Approach*. John Wiley and Sons.
- 3. Yadav, L. D. S., Singh, J., and Singh, J. (2017). *Organic Synthesis*, Pragati Prakashan, India.
- 4. Norman, R.O.C., and Coxon, J. M. (1993). *Principle of Organic Synthesis*, CRC Press; 3rd edition.
- 5. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*. Narosa Publishing House (P) Ltd., New Delhi.
- 6. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.

- 7. Bansal, R. K. Heterocyclic Chemistry, 5thEdition, 2010, New Age International (P) Ltd., New Delhi.
- 8. Carey, F. A., and Sundberg, R. J. (2007). Advanced organic chemistry: part B. Springer Science and Business Media.
- 9. Finar, I. L. (1996). *Textbook of Organic Chemistry. ELBS*, Pearson Education UK.
- 10. Gilchrist, T. L., (1997). *Heterocyclic Chemistry*. Addison Wesley Longman Publishers, US.
- 11. Gupta R.R., Kumar M., and Gupta V., (2010). Heterocyclic Chemistry—II Five Membered Heterocycles. Vol. 1–3, Springer Verlag, India.
- 12. Joule, J. A., and Mills, K., (2010). *Heterocyclic Chemistry*. Blackwell Publishers, New York.
- 13. Smith, M. B., (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*. John Wiley and Sons.
- 14. Corey, E. J., and Cheng X.-M., (1989). The Logic of Chemical Synthesis. John Wiley and Sons.
- 15. Gulevich, A. V., Dudnik, A. S., Chernyak, N., and Gevorgyan, V., *Transition Metal-Mediated Synthesis of Monocyclic Aromatic Heterocycles.* Chemical Reviews, 2013, 113, 3084-3213.
- 16. Patil, N. T., and Yamamoto, Y., Coinage Metal-Assisted Synthesis of Heterocycles. Chemical Reviews, 2008, 108, 8, 3395-3442.
- 17. Gribble, G. W., Joule J. A. (2021) Progress in Heterocyclic Chemistry, Elsevier Health Sciences Division, USA

Course Title: Bioinorganic and Biophysical Chemistry

Paper Code: CHM.553
Total Contact Hours: 45

L	Т	P	Cr
3	0	0	3

Learning Outcome: At the end of this course student will be able to

- Determine structure and biological functions of metalloproteins and enzymes.
- Classify metallobiomolecules on the basis of their functional properties.
- Analyze the role of metal ions in the biological system.
- Determine the factors that govern the thermodynamic and mechanical stability, folding, and dynamics of proteins.
- Interpret kinetics, thermodynamics, and mechanism of protein folding.

Unit 1 Hours Inorganic Chemistry of Enzymes – I: Metalloporphyrins: Hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, structure and function of hemoglobin and myoglobin. Other iron-porphyrin biomolecules, peroxidases and catalases, cytochromes, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer. Biochemistry of iron, iron storage and transport, ferritin and transferrin.

Brainstorming regarding structure-function relationship of heme and non-heme protein.

Unit 2 Hours

Inorganic Chemistry of Enzymes – II: Metallothioneins: Ferredoxins, carboxypeptidase, carbonic anhydrase, blue copper proteins, superoxide dismutase and hemocyanins.

Enzymes: Structure and function, inhibition and poisoning vitamin B_{12} and B_{12} coenzymes metallothioneins, bio-inorganic chemistry of Mo and W. Comparison of the reactivity of Ferredoxins and artificial Iron-sulfur clusters.

Peer group discussion on structure-function relationship of metallothioneins and metalloenzymes.

Unit 3 Hours

Metal Ions in Biological Systems: Role of metal ions in replication and transcription process of nucleic acids. Biochemistry of calcium as hormonal messenger, muscle contraction, blood clotting, neurotransmitter, metals in the regulation of biochemical events.

Group discussion on the significance of metal ions and non-metals in various diseases.

Unit 4
Hours

Biophysical Chemistry: Principles of biophysical chemistry (pH, buffer, reaction kinetics, thermodynamics), physical principle of structure, function, and folding of proteins, conformations of proteins (Ramachandran plot, secondary, tertiary and quaternary structure; domains; motif and folds), determination of protein structures by spectroscopic methods (CD, FTIR, NMR), thermodynamics of protein folding by spectroscopic and calorimetric methods, protein conformational study by NMR and fluorescence spectroscopy.

Demonstration of applications of spectroscopic and calorimetric techniques for biochemical and biophysical characterizations of macromolecules.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial.

Suggested Readings

- 1. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic chemistry: Principles of Structure and Reactivity.* Pearson Education India.
- 2. Douglas, B. E., and McDaniel, D. H. (1965). Concepts and models of inorganic chemistry. John Wiley and Sons.
- 3. Cotton, F. A., and Wilkinson, G. (1988). *Advanced inorganic chemistry* (Vol. 545). New York: Wiley.
- 4. Elschenbroich, C. (2016). Organometallics. John Wiley and Sons.
- 5. Atkins, P., Overtone, T., Rourke, J., Weller, J., and Armstrong, F., (2010). *Shriver and Atkins' inorganic chemistry*. Oxford University Press.
- 6. Cowan, J. A. (1997). *Inorganic Biochemistry: An Introduction*. Wiley VCH.
- 7. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vol. 18, Wiley-Interscience.
- 8. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vol. 38, Wiley-Interscience.
- 9. Lesk, A. M., (2010). *Introduction to Protein Science: Architecture, Function, and Genomics.* Oxford University Press.
- 10. Cantor, C. R. and Schimmel, P. R., (1980). *Biophysical Chemistry*. Freeman.
- 11. Van Holde, K. E., Johnson, W.C., and Ho, P. S., (2006). *Principles of Physical Biochemistry*. Pearson Education.
- 12. Harding, S. E. and Chowdhry, B. Z. (2001). *Protein-Ligand Interactions*. Oxford University Press.
- 13. Kepp, K. P., Bioinorganic Chemistry of Alzheimer's Disease. Chemical Reviews 2012, 112, 10, 5193-5239.
- 14. Snyder, B. E. R., Bols, M. L., Schoonheydt, R. A., Sels, B. F. and Solomon, E. I. Iron and Copper Active Sites in Zeolites and Their Correlation to Metalloenzymes. Chemical Reviews 2018, 118, 2718–2768.
- 15. Huang, X., and Groves, J. T., Oxygen Activation and Radical Transformations in Heme Proteins and Metalloporphyrins. Chemical Reviews, 2018, 118, 2491-2553.

Course Title: Applied Electrochemistry	L	Т	P	Cr
Paper Code: CAC.554	3	0	0	3

Total Lectures: 45

Learning Outcome: Upon completion of the course the student would be able to

- Elucidate the working and efficiency of Commercial electrochemical cells and Mechanism of Corrosion.
- Demonstrate and apply electrochemistry of bio/chemical origin in analysis of important analytes of biological relevance.

Unit I Hours

Conversion and storage of electrochemical energy, maximum intrinsic efficiency of an electrochemical converter. physical interpretation of the Carnot efficiency factor in electrochemical energy converters. power outputs. Electrochemical generators (fuel cells): hydrogen oxygen cells, hydrogen air cell, hydrocarbon air cell, alkaline fuel cell, applications of fuel cells.

Brainstorming approaches to enhance efficiency of fuel cell and electrochemical devices.

Unit II Hours

Electrochemical energy storage. Properties of electrochemical energy storage: measure of battery performance, charging and discharging of a battery, Classical batteries: (i) lead acid (ii) nickel-cadmium. Modern batteries: (i) nickel-metal hydride, (ii) lithium battery.

Efficiency of energy storage devices through peer learning. Hands-on model building of electrochemical devices based on sustainable national policies.

Unit III Hours

Corrosion and stability of metals. Mechanism of the corrosion of the metals; thermodynamics and the stability of metals, corrosion current and corrosion potential -Evans diagrams. Measurement of corrosion rate: Inhibiting corrosion, Passivation. Structure of passivation films, mechanism of passivation.

Brainstorming the corrosion of metals and passivation technologies of the current world.

Unit IV 11Hours

Bioelectrochemistry. Bioelectronics, membrane potentials, simplistic theory, modern theory, electrical conductance in biological organisms: enzymes as electrodes. kinetic of electrode process. Essentials of electrode

reaction. Current density, overpotential, Tafel equation, Butler Volmer equation.

Applications of bio/chemical electrochemistry for sensing analytes of medical relevance through peer learning.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

- 1. Mabbott, G. A., (2020) Electroanalytical Chemistry: Principles, Best Practices, and Case Studies, Wiley Publishers.
- 2. Ozkan, S.A., Kauffmann, J.-M., Zuman, P., Brett, A. M. O. (2015) Electroanalysis in Biomedical and Pharmaceutical Sciences: Voltammetry, Amperometry, Biosensors, Applications, Springer Berlin Hidelberg.
- 3. Garche, J., and Moseley, P. T. (2014) Electrochemical Energy Storage for Renewable Sources and Grid Balancing, Elsevier Science.
- 4. Ezema, F. I., and Kebede, M. A. (2019) Electrochemical Devices for Energy Storage Applications, CRC Press.
- 5. Hester, R. E., and Harrison, R. M. (2018) Energy Storage Options and Their Environmental Impact, RSC Publishing.
- 6. Job, R. (2020) Electrochemical Energy Storage: Physics and Chemistry of Batteries, DeGruyter Publishers. Bockris, J. O. M., and Reddy, A. K. (1998). Modern Electrochemistry 2B: Electrodicsin Chemistry, Engineering, Biology and Environmental Science (Vol. 2). Springer Science and Business Media.
- 7. Srinivasan, S., (2006). *Fuel Cells: From Fundamentals to Applications*. Springer Science + Business Media LLC.
- 8. Bond, A. M. (1980). Modern Polarographic Methods in Analytical Chemistry (Vol. 4). CRC Press.
- 9. Zutshi, K. (2006). Introduction to Polarography and Allied Techniques. New Age International.
- 10. Monk, P. M. S., (2001). Fundamentals of Electroanalytical Chemistry. Wiley and Sons.
- 11. Vassos, B. H., and Ewing, G. W., (1983). *Electroanalytical Chemistry*. Wiley Interscience.
- 12. Scholtz, F. (2013) Electroanalytical Methods: Guide to Experiments and Applications Springer Berlin Heidelberg.

Course Title: Organic Synthesis and Catalysis L T P Cr	Course Title: Organic Synthesis and Catalysis	L	Т	P	Cr
--	---	---	---	---	----

Paper Code: CAC.559		3	0	О	3	
---------------------	--	---	---	---	---	--

Total Contact Hours: 45

Learning Outcomes: The students will be able to

- Design various molecules of commercial and biological importance using modern cross-coupling strategies and organometallic compounds.
- Understand and apply asymmetric transformations for the synthesis of chiral compounds.
- Know the use of various reagents and various name reaction for the small scale fine chemical synthesis.

Unit 1 Hours

Synthetic reactions and their applications: Baylis-Hillman reaction, Biginelli reaction, Mukaiyama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's stereoselective olefination, Buchwald-Hartwig coupling, Eishenmosher-Tanabe fragmentation and Shapiro reaction, Stork-enamine reaction, Aza-Cope, Aza-Wittig reaction, Ugi reaction, Robinson-Gabriel synthesis, Vilsmeier-Haack reaction.

Latest advancement including green aspects of various name reactions and their industrial applications through group presentation.

Unit 2 11 Hours

Asymmetric synthesis: Chiral pools, chiral catalysis: chiral auxiliaries, methods of asymmetric induction — substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. resolution — optical and kinetic, chemoregio— and stereoselective transformations, organocatalysis and biocatalysis. Reactions using chiral Lewis and Bronsted acids.

Purpose and importance of chirality in various biologically active compounds and drug molecules (recent stringent FDA guidelines regarding chiral drugs) through brainstorming.

Unit 3 11 Hours

Metal Catalysis and Cross coupling reactions

Palladium catalyzed chemistry for C-C bond formation reaction, Heck coupling, Sonogashira coupling, Suzuki-Miyaura coupling, Negishi

coupling; C-N bond formation reactions, copper catalyzed chemistry, synthesis *via* C-H activation, metal catalyzed reactions under microwave conditions, Solid supported reactions, Multicomponent reactions, Click Chemistry.

Application towards synthesis of fine chemicals

Peer group learning through presentation on the Industrial applications of various cross-coupling reactions for the synthesis of value added chemicals.

Unit 4 Hours

Organometallic compounds and their applications: Organoboranes: Preparation of organobornaes viz hydroboration with BH₃-THF, dicyclohexylborane, disiamylborane, thexylborane, 9-BBN, Chiral organoboranes and their utility: diisopinocampheyl borane, alpine boranes. Metal catalysed hydroboration, functional group transformations of organo boranes: oxidation, protonolysis and rearrangements. formation of carboncarbon-bonds *viz* organoboranes carbonylation.

Organolithium, organozinc, organosilicon, and, organocopper compounds (Gilman reagent) and their applications for fine chemical synthesis.

Expression of the views of the students on latest advancement in the area of organoboranes including stereochemical aspects through presentation.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Li, J. J., (2021). Name Reactions: A Collection of Detailed Reaction Mechanism. Springer; 6th edition.
- 2. Kalsi, P. S. (2020). *Organic Reactions and Their Mechanism*. New Age International Publisher, India; 5th edition.
- 3. Finar, I.L., (2012). Organic Chemistry. Pearson Education, UK.
- 4. Smith, M. B., (2020). March's Advanced Organic Chemistry: Reactions, Mechanisms, And Structure. John Wiley and Sons.
- 5. Corey, E.J. and Cheng, X.-M. (2011). *The Logic of Chemical Synthesis*. John Wiley and Sons.
- 6. Davies, S. G., (2013). Organotransition Metal Chemistry: Applications to Organic Synthesis: Applications to Organic Synthesis (Vol. 2). Elsevier.

- 7. Aitken, A., and Kilényi, S. N., (Eds.). (2012). Asymmetric Synthesis. Springer.
- 8. Mundy, B. P., Ellerd, M. G., and Favaloro Jr, F. G., (2005). *Name Reactions and Reagents in Organic Synthesis*. John Wiley and Sons.
- 9. Sacramento, M., Costa, G. P., Barcellos, A. M., Perin, G., Lenardão, E. J., & Alves, D. (2021). Transition-metal-free C-S, C- Se, and C- Te Bond Formation from Organoboron Compounds. The Chemical Record.
- 10. Schettini, R., & Della Sala, G. (2021). New Trends in Asymmetric Catalysis. *Catalysts*, 2021, 11, 306.
- 11. L Budarin, V., S Shuttleworth, P., H Clark, J., & Luque, R. (2010). Industrial applications of CC coupling reactions. *Current Organic Synthesis*, 7(6), 614–627.

Course Title: Environmental Chemistry	L	Т	P	Cr
Paper Code: CAC.560	3	0	0	3

Total Lectures: 45

Learning Outcome: The student will be able to

- Elucidate the understanding of the various physiochemical processes in air, water and soil environment.
- Application of various physicochemical parameters in the modelling and predicting the movement of a pollutant in environment.
- Elucidate the understanding of the various policies in environment.
- Elucidate and apply chemistry in water/wastewater treatment.

Unit 1 12 Hours

Aquatic chemistry: Surface, ground water, marine and brackish water resources – assessment and utilization; Rivers and Lakes in India; hydrological cycle; Structure and properties of water, Water quality parameters, Physicochemical concepts of colour, odour, turbidity, pH, conductivity, DO, COD, BOD and its kinetics, Carbonates and alkalinity, redox potential, Pourbiax diagram, pH-pE diagrams for Iron, oxoanions and anions,

Environmental Issues: Ground water depletion; Water logging and salinity; Water Conservation and management techniques; Rain water harvesting;

Watershed management; Eutrophication; Restoration of Lakes, transboundary river water sharing and interlinking of rivers.

Water parameters and water issue correlation by peer learning.

Unit 2
Hours

Interfacial Interactions: Environmental chemistry of arsenic, chromium, Chemical potential, fugacity and its application to fugacity model.

Water treatment Technologies: Chemical and Physical Methods of wastewater treatment with emphasis on sedimentation, coagulation, adsorption, water softening, defluoridation and ion exchange process.

Biological wastewater treatment including Activated sludge process, trickling filter and Membrane bioreactor, biological treatment processes – process description, design and application.

Field visit to water treatment plants in municipal and industrial Water treatment technologies.

Unit 3 11 Hours

Membrane Processes: Reverse Osmosis, Types of membrane, characterization of membranes, nano-membranes and their formation, efficiency of different membranes in removal of different elements.

Atmospheric chemistry: Composition of air, Chemical speciation, particles, ion and radicals, Formation of particulate matter, Photochemical reactions in the atmosphere, Chemistry of air pollutants, Photochemical smog, Acid rain, Ozone Chemistry and Montreal Protocol, Greenhouse gases and Global warming, Clean Development Mechanism and Kyoto Protocol, Persistent Organic Pollutants (POP) and Stockholm Convention.

Understanding the international, national and local response to issues related to air/water through brainstorming.

Unit 4
Hours

Chemistry of Soil: Physio-chemical composition of soil, humus, inorganic and organic components of soil, nutrients (NPK) in soil, significance of C: N ratio, cation exchange capacity (CEC), reactions in soil solution, ion exchange (physiosorption), ligand exchange (chemisorption), complexations, chelation; precipitation / dissolution.

Sources of Natural and Artificial Radiations: Dosimetry, types of dosimeters, radioactive substances, applications and handling of isotopes and other radionuclides in environment.

Biochemical and Toxicological aspects of arsenic, cadmium, lead, mercury, carbon monoxide, O₃, PAN, MIC and other carcinogens.

Understanding the radioactive safety management and toxicology through field visit and peer learning, respectively.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

- 1. Trimm, H. H., and Hunter, W. (2021) Environmental Chemistry: New Techniques and Data, Taylor and Francis Group.
- 2. Muhammad A. Hanif, M. A., Nadeem, F., Bhatti, I. A., Tauqeer H. M. (2020) Environmental Chemistry: A Comprehensive Approach, Wiley Publishing.
- 3. Bleam, W. F. (2016) Soil and Environmental Chemistry, Elsevier Science.
- 4. Baird, C., and Cann, M., (2008). Environmental Chemistry. W.H. Freeman, USA
- 5. Manahan, S. E., (2008). Fundamentals of Environmental Chemistry. CRC Press, USA
- 6. Connell D. W. (2005). Basic concepts of Environmental Chemistry, CRC Press, USA
- 7. Girard, J., (2010). Principles of Environmental Chemistry. Barlett Publishers, USA.
- 8. Harrison, R. M., (2007). Principles of Environmental Chemistry. RSC Publishing, UK
- 9. Grady Jr, C. L., Daigger, G. T., Love, N. G., and Filipe, C. D. (2011). *Biological Wastewater Treatment*. CRC Press.
- 10. Hillel, D., (2007). Soil in the Environment: Crucible of Terrestrial Life. Academic Press, USA.
- 11. Manahan, S. E., (2010). Water Chemistry: Green Science and Technology of Nature's Most Renewable Resource. CRC Press, USA.
- 12. Tchobanoglous, G., Burton, F. L., and Stensel, H. D., (2003). *Wastewater Engineering: Treatment and Reuse*. McGraw-Hill Science, USA.
- 13. American Public Health Association, American Water Works Association and Water Environment Federation, (2005). *Standard Methods for the Examination of Water and Wastewater*. American Public Health Association.
- 14. Eckenfelder, Jr., W.W., Ford, D.L., and Englande, A.J., Jr. (2009). *Industrial water quality*. McGraw-Hill.

- 15. Crittenden, J. C., Trussell, R. R., and Hand, D. W., (2005). *Water treatment: principles and design*. Wiley Publishers, USA.
- 16. Stockholm Convention, http://www.pops.int/.
- 17. United Nation Framework Convention on Climate Change, https://unfccc.int/ and https://unfccc.int/ and https://unfccc.int/kyoto_protocol.

Course Title: Applied Polymer Chemistry	L	Т	P C	r
Paper Code: CAC.571	3	0	0 3	

Total Lectures: 45

Learning Outcomes: The student upon completion of the course would be able to

- Elucidate the different mechanisms of polymerization.
- Apply the various methods for determination of Number, weight and viscosity averaged molecular weights.
- Elucidate and demonstrate the processing of thermoplastic and thermosetting polymers.
- Apply the polymers for their use in biological and lifestyle applications.

UNIT I 13 Hours

Polymers Synthesis and Characterization: Classification of polymers. Types of polymerization processes: Bulk, solution, suspension and emulsion polymerization, their advantages and disadvantages. Addition, radical, ionic, coordination and condensation polymerisation; their mechanism and role of initiator, chain transfer agent, solvent and inhibitor. Effect of structure of monomer on free-radical polymerization. Polymerisation conditions and polymer reactions. Polymerisation in homogeneous and heterogeneous systems. Method for reaction rate determination using Rotating disk method and Pulsed Laser Photolysis – Size exclusion chromatography (PLP-SEC).

UNIT II 11 Hours

Polymer: Significance of molecular weight of polymer. Polydispersive average molecular weight. number, weight and viscosity average weights. Measurement of molecular weights. End group, viscosity, light scattering, osmotic and ultracentrifugation methods. Chemical and spectroscopic analysis of polymers. X-ray diffraction study.

Structure and properties: Configuration of polymer chains. Crystal structure of polymers, morphology of crystalline polymers. Thermal analysis, tensile strength, fatique, impact, tear resistance, hardness and abrasion resistance. Understanding of molecular weight characteristics of polymer would be carried out through problem solving. The effect of the polymer molecular weight and crystallinity on mechanical properties would be understood though peer learning.

UNIT III 11 Hours

Polymer structure and physical properties: crystalline melting point T_m , melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g relationship between T_m and T_g , effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking.

Polymer Processing: Plastics, elastomers and fibres. Compounding. Processing techniques, calendaring, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

Factors responsible for the polymer processing would be brainstormed for shaping polymers.

UNIT IV 10 Hours

Applications of Polymers: Properties of polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers, fire retarding polymers and electrically conducting polymers. Biomedical polymers, contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

Biopolymers: The structure, function, and properties of synthetic (dextran, ficoll) and natural biopolymers (Cellulose, CMC, alginate, chitin, DNA, nucleic acids, nucleotides, proteins), conformation of nucleic acids (DNA, t-RNA, micro-RNA), molecular architecture for some biological structures such as collagen, tissue, silk, wool, and shell. Introduction to biomedical materials and drug delivery formulations.

Understanding the limitations to sustainable polymer use through peer learning. Brainstorming session on biomedical applications in drug delivery and blood.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

Suggested Readings

1. Billmeyer, Jr., F.W. (2007). Textbook of Polymer Science. Wiley.

- 2. Odian, G. (2004). Principles of Polymerization. John Wiley and Sons.
- 3. Cowie, J. M. G., and Arrighi, V. (2007). *Polymers: Chemistry and Physics of Modern Materials*. CRC press.
- 4. Takemoto, K. Inaki Y. and Ottanbrite R.M. (1997). Functional Monomers and Polymers, CRC Press.
- 5. Gowariker, V. R., Viswanathan, N. V., and Sreedhar, J. (1986). *Polymer Science*. New Age International.
- 6. Alcock H.R., Lambe, F.W., and Mark, J. E., (2003). *Contemporary Polymer Chemistry*, Prentice Hall.
- 7. Peacock, A., and Calhoun, A. (2012). *Polymer Chemistry-Properties and Applications*. Hanser Publishers, Munich.
- 8. Chandra, R., and Adab, A., (1994). *Rubber and Plastic Waste*. CBS Publishers and Distributors, New Delhi,
- 9. Bahadur, P., and Sastry, N. V., (2002). *Principles of Polymerisation*, Narosa Publishing House, New Delhi.
- 10. Thomas, E. (2007) https://ocw.mit.edu/courses/materials-science-and-engineering/3-063-polymer-physics-spring-2007
- 11. Langbeheim, E. (2020) Simulating the Effects of Excluded-Volume Interactions in Polymer Solutions J. Chem. Educ. 97(6), 1613-1617 DOI: 10.1021/acs.jchemed.0c00003

Course Title: Green and Industrial Organic Chemistry		L	Т	P	Cr
Paper Code: CAC.572		3	0	0	3

Total Lectures: 45

Learning Outcomes: At the end of the course student will be able to

- Design a reaction scheme taking into consideration its green and economical aspects
- Identify various industrial manufacturing processes for value added chemicals.
- Realize the importance of green chemistry and to apply various tools of green chemistry in their future research.

Unit 1
Hours

Green Chemistry: Principles of green chemistry, atom economy, tools of green chemistry: green solvents (ionic liquids, supercritical fluids), abundant natural feedstocks/starting precursor, multicomponent reactions (MCRs), tandem/domino reactions, microwave assisted organic synthesis

(MAOS), solid phase synthesis, aqueous media reactions, General introduction to Combinatorial Chemistry.

Recyclability of ionic liquids through demonstration. Industrial applications of green solvents: peer discussion in the classroom

Unit 2 Hours

Applications of Green Chemistry: Green synthesis of ibuprofen, design and use of CO₂-surfactants for precision cleaning in industries, environmentally preferable marine antifoulant, use of molting accelerators in place of toxic and harmful insecticides, oxidant activators to replace chlorine-based delignification process in paper and pulp industry, green chemistry process for polyester regeneration, Biocatalytic promiscuity of enzymes for C-C bond formation. Recent applications of ionic liquids as solvent and catalysts in the chemical industry.

Various green processes employed in chemical industries through group presentation.

Unit 3 11 Hours

Industrial Organic Syntheses: The raw material and basic processes, chemical processes used in industrial organic synthesis: production of methanol, ethanol, ethyl acetate, ammonia, sulphuric acid, acetaldehyde, acetic acid, ethylene glycol, glycerine, acetone, phenol, formaldehyde, 1,3-butadinene and styrene.

Unit4 11 Hours

Detergent: Introduction, Principal groups of synthetic detergents, Classification of surfactants; anionic, cationic, amphoteric and non-ionic detergents, alkyl/aryl/ amide sulphonates, binders and builders, fillers, ecofriendly detergents: detergents containing enzymes and zeolites. Oleochemicals as source for surfactants: Methyl ether sulfonate (MES).

Project work on the types of various detergents/surfactants present at home and their specific utility.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

Suggested Readings:

- 1. Anastas, P. T., and Warner, J. C. (2000). *Green chemistry: theory and practice*. Oxford university press.
- 2. Sauer, N. N. (2000). *Green Chemistry: Frontiers in Benign Chemical Syntheses and Processes* Ed. Anastas P. T. and Williamson T. C., (US Environmental Protection Agency). Oxford University Press: New York, NY.
- 3. Malhotra, S. V. (2007). *Ionic Liquids in Organic Synthesis*, Oxford University Press, US.
- 4. Weissermel, K., and Arpe, H.J., (2010) *Industrial Organic Chemistry*. Wiley-VCH.
- 5. Sheldon, R.A., Arends, I., and Hannefed, U., (2007). *Green Chemistry and Catalysis*. Wiley-VCH Verlag GmbH and Co.
- 6. Ahluwalia, V.K and Kidwai, M. (2012) *New Trends in Green Chemistry*. Springer.
- 7. Scragg, A.H. (2009) Biofuels: Production, Application and Development, CAB International, UK.
- 8. Gupta, A.K., (2021) Modern Technology of Soaps, Detergents and Toiletries (With Formulae and Project Profiles) 2Nd Edition
- 9. Gaudino, E. C., Cravotto, G., Manzoli, M., & Tabasso, S. (2019). From waste biomass to chemicals and energy via microwave-assisted processes. *Green Chemistry*, 21(6), 1202–1235.
- 10. Clauser, N. M., González, G., Mendieta, C. M., Kruyeniski, J., Area, M. C., & Vallejos, M. E. (2021). Biomass waste as sustainable raw material for energy and fuels. *Sustainability*, 13(2), 794.
- 11. Plechkova, N. V., & Seddon, K. R. (2008). Applications of ionic liquids in the chemical industry. *Chemical Society Reviews*, 37(1), 123–150.

L	Т	P	Cr
3	0	0	3

Course Title: Industrial Inorganic Chemistry

Paper Code: CAC.573 Total Lectures: 45

Learning Outcome: The students will be able to

- Elucidate the understanding of the semiconductors and electronics made from inorganic materials.
- Elucidate the manufacturing of various fertilizers, electroplating processes and glasses and ceramics.

Unit-I

10Hours

Special Materials for Electronic Industry Recent trends in sensor technology, film sensors, Semiconductor IC technology, micro-electro mechanical systems (MEMS), nanosensors. Applications of Sensors: automobile sensors, home appliance sensor, aerospace sensors, sensors for manufacturing medical diagnostic sensors, sensors for environmental monitoring. High purity silicon, germanium, gallium arsenide (GaAs), indium phosphide (InP) etc. Preparation using zone refining, crystal growth and there use in electronic industry. High temperature materials, SiC, chromite, alumina, zirconia, magnesite etc. Ionic and superionic conductors, β alumina oxide ion conductors, halide conductors superionic, fast ion conductors- RbAg₄I₅.

Group Discussion on sensors applications in current scenario.

Unit-II 15 Hours

Fertilizer Industries. General principles of plant nutrition: essential plant nutrients, functions of the essential elements, classification of commercial nitrogenous fertilizers. Manufacturing of ammonium sulphate, urea, ammonium nitrate, commercial phosphatic fertilizers. Manufacturing process and properties of phosphatic fertilizers, single super phosphate, triple super phosphate. Commercial potassic fertilizers: chemicals of potassium compounds, classification, manufacturing process and properties potassium fertilizer, potassium sulphate, mixed of fertilizer. Micronutrients: role and deficiency symptom of micronutrients. Biofertilizers: classification, demands and production, present status of fertilizer industries in India.

Demonstration on industrial scale synthesis of various fertilizers and use of fertilizers and pesticides in agriculture.

Unit-III 10Hours

Metal Finish Technology. Basics of electrodeposition, electroplating principles and practice, electrochemistry applied to electroplating, electroplating of metals chromium, cadmium, nickel, copper, silver, gold, purpose of metal electroplating composition and condition of plating bath, applications waste treatment and metal recovery.

Peer discussion on electroplating techniques of different transition metals and their applications in water treatment.

Unit-1V 10Hours

Glass and Ceramics. Physical and chemical properties of glasses, raw materials, manufacturing of special glasses. Ceramics and their properties, raw materials, manufacturing of ceramics, applications of colours to pottery, use of ceramics. Industrial gases: manufacturing and industrial uses of H₂, O₂, N₂, CO₂, Cl₂and acetylene gases. Liquefaction of gases, production of low temperature. Chemicals of utility: inorganic fine chemicals, magnesia, alumina, AlCl₃, calcium carbonate, sodium silicate, MnO₂, FeSO₄, PbO₂ and NaOH.

Brainstorming session on generation of differ gas techniques with safety features.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

Suggested Readings

- 1. Keer, H. V. (1993). Principles of the solid state. New Age International.
- 2. West, A. R. (2003). *Solid State Chemistry and its applications*. John Wiley and Sons.
- 3. Sharma, B. K. (2014). Engineering chemistry. Krishna Prakashan Media.
- 4. Lowenheim, F. A., (1978). Electroplating, MC Graw-Hill Book Company.
- 5. Gable, D., (1978). Principal of metal Treatment and protection. Pergaman Press Oxford
- 6. Burke, J. E., (1966). Progess in ceramic scienceVol. IV. Pergamon Press.
- 7. Ash, M. and Ash I., (2000). Formulary of paints and other coating. Vol. I, Chemical Punlising Press.
- 8. Sharma, B. K., (1997). Industrial Chemistry, Goel Publishing House.
- 9. Shukla S. D. and Pandey, G. N. (1979). A text book of chemical technology. Vikas Publishing House.
- 10. Henglein, F. A. (2013). Chemical technology. Elsevier.
- 11. Patranabi, D. (2003). Sensors and Tranducers. PHI Learning Pvt. Ltd
- 12. Basak, R. K. (2009). Fertilizers: A Textbook, Kalyani Publishers.
- 13. Balasubramaniam, R. (2009). Callister's Materials Science and Engineering: Indian Adaptation (W/Cd). John Wiley and Sons.

Course Title: Dyes and Pigments	L	Т	P	Cr
Paper Code: CAC.575	3	0	0	3

Total Contact Hour: 45

Learning Outcome: Upon successful completion of the course the student will be able to apply the knowledge of

- Synthetic and natural dyes in various fields.
- Synthetic and natural pigments in various fields.
- Analysis and physical properties of pigments and dyes

Unit 1 11 Hours

Introduction of pigments: Colour index, generic names of pigments, colour constitution number, polymorphism, properties required in a pigment and extender, dyes, pigment dyestuffs, and hue of the pigment (Bathochromic and hypsochromic shift), practices and requirement of pigments. Organic pigments – Antraquinone, Benzimidazolone dioxazines, Diazo lakes, Litholrubones, Monoazo lakes, Naphthol AS lakes, Naphthol AS, Perylenes, Phthalocyanines, Quinacridones effect pigments and biological pigments.

Different structures and properties of pigments through peer learning Group project on synthesis of azo pigments

Unit 2 Hours

Classification and synthesis of dyes: Colour theory of dyes, Various unit operations in the manufacture of intermediates and dyes, Introduction of various functional groups, synthesis of dyes, basics of azo dyes, diazotization and coupling reactions, azoic colours; vat dyes, reactive dyes, acid dyes, mono azo dye; diasazo, nitro, diphenylamine and anthraquinone dyes; acid mordant dyes, azo metal complex dyes, synthesis of different dyes. Nylon, Polyesters and Polyamides structures and names of dyes applied on each of them.

Class room debate on colour theory of dyes Group presentation on synthesis of various dyes

Unit 3 12 Hours

Processing and synthesis of inorganic pigments and Raw materials for organic pigments: Crushing and grinding, vaporization, co-precipitation, filtration, drying, flushing, calcinations/roasting, vapour phase oxidation etc. Pigments Extenders: Sources, manufacture, properties and uses of carbonates, sulphates and other extender pigments. White prime pigments: Methods of manufacturing, comparison of properties and composition of TiO2, ZnO, Zinc sulphide and lithopone, Surface treatment of TiO2 and other pigments, A brief study of coal tar distillation and the role of distillation products in the manufacture of synthetic dyes: bases and precipitants used in the colour striking.

Unit 4
Hours

Analysis of Dyes and Pigments:

Analysis of Dyes & Intermediates: Colour fastness, Light fastness, sublimation fastness, Paper Chromatography, Thin Layer Chromatography, Column Chromatography, Colour Matching Spectrophotometer, UV-visible Spectrophotometer.

Analysis of Pigments: Crystal structure, particle size, shape and distribution, refractive index and hiding power, oil absorption, specific gravity, bulking value, reducing power, tinting strength, fastness properties such as resistance to light, heat, water, chemicals, bleeding etc. corrosion resistance, toxicity of pigments etc.

Group projects on role of dyes and pigments in paint industries Peer learning on the importance of dyes in biological perspective

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Zollinger, H. (2003). Colour Chemistry: Syntheses, Properties, and Applications of Organic Dyes and Pigments. John Wiley and Sons.
- 2. Venkataraman, K. (Ed.). (2012). The Chemistry of Synthetic Dyes (Vol. 4). Elsevier.
- 3. Buxbaum, G. (Ed.). (2008). *Industrial Inorganic Pigments*. John Wiley and Sons.
- 4. Herbst, W., and Hunger, K. (2006). *Industrial Organic Pigments: Production, Properties, Applications.* John Wiley and Sons.
- 5. Januschewski, E., Bischof, g., Thanh, B. n., Bergmann, P., Jerz, g., Winterhalter, P., Heinz, V., Juadjur, A. Rapid UV/Vis Spectroscopic Dye Authentication Assay for the Determination and Classification of Reactive Dyes, Monascus Pigments, and Natural Dyes in Coloring Foodstuff, J. Agric. Food Chem. 2020, 68, 42, 11839–11845.
- 6. Silva, G. t. M., Silva, K. M., Silva, C. P., Gonçalves, J. M., Quina, F.H. Hybrid Pigments from Anthocyanin Analogues and Synthetic Clay Minerals, *ACS Omega* 2020, 5, 41, 26592–26600.

Course Title: Petroleum Chemistry	L	Т	P	Cr
Paper Code: CAC.576	3	0	O	3

Total Lectures: 45

Learning Outcomes: The student will have knowledge for

- Identifying energy sources and use of mankind
- Workout on renewable sources of energy and sources.
- Address the issues related to various energy alternatives.

Unit 1 11

Hours

Petroleum Refining: Fossil fuel and origin of petroleum, Petroleum resources: detection and exploration of petroleum. Nature of extracted crude oil, classification of crude oil, Physicochemical characteristics of crude oil. General processing of crude oil – Fractionation (atmospheric and vacuum) and stripping, solvent method, de-asphalting, Refining.

Brainstorming on various energy resources

Various processes for the economic isolations of petroleum based products: Peer group learning

Unit 2 11

Hours

Cracking process: thermal and catalytic. Blending of gasoline, knocking and Octane rating, gasoline additives for Aviation fuel. Diesel oil, Cetane rating, Kerosene. LPG-Composition and uses. Synthetic petrol (Fischer-Tropsch method). Desulphurization and denitrogenation of gasoline.

Group presentation on the recent advances on Desulphurization and denitrogenation of gasoline.

Unit 3 11 Hours

Petroleum Speciality Products: Raw materials for aliphatic, and inorganic petrochemicals. hydrocarbon solvents, petroleum derived pesticides, refrigeration gases, lubricants and waxes, carbon black, petroleum coke. Methyl tert-butyl ether, polyvinyl acetate, polyvinyl chloride, Teflon, polythene, polypropylene, ethylene, propylene elastomers; Oxo-process.

Brainstorming on the use of various petroleum speciality products used at home.

Unit 4 12

Hours

Petroleum as a raw material for aromatic petrochemicals: Caprolactam, polystyrene, terephthalates. Cumene process (Hock process): phenolacetone production.

Chemicals and products from natural gas: Syn-gas, methanol, ammonia; Ammonia-Urea plant; Fertilizer.

Group presentation on various recent processes using petroleum based feedstocks for the synthesis of aromatic compounds.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

- 1. Curley, R., (2011). Fossil Fuels Energy: Past, Present, and Future. Rosen Education Service.
- 2. Richards, J. (2009). Fossil Fuels. Benchmark Books.
- 3. Solway, A., (2007). Hydrogen Fuel Energy for the Future and Global Warming. Gareth Stevens Publishing.
- 4. Scheer, H., (2012). Energy Autonomy: The Economic, Social and Technological Case for Renewable Energy. Routledge.
- 5. Simon, C. A., (2007). Alternative Energy: Political, Economic, and Social Feasibility. Rowman and Littlefield Publishers Inc.
- 6. Karim, G. A., (2013). Fuels, Energy, and the Environment. CRC Press.
- 7. Luque, R., and Melero J. A., (2012). Advances in Biodiesel Production: Processes and Technologies. Woodhead Publishing.
- 8. Basu, P., (2013). Biomass Gasification and Pyrolysis: Practical Design and Theory. Academic Press.
- 9. Klass, D. L. (1998). Biomass for Renewable Energy, Fuels, and Chemicals.
- 10. Fahim, M., Al-Sahhaf, T., and Elkilani, A. (2009). Fundamentals of Petroleum Refining. Elsevier.
- 11. Luque, R., Campelo, J., and Clark, J., (2010). Handbook of Biofuels Production: Processes and Technologies. Woodhead Publishing.
- 12. Speight, J. G. (2019). Handbook of petrochemical processes. CRC Press.
- 13. Kulprathipanja, S., Rekoske, J. E., Wei, D., Slone, R. V., Pham, T., & Liu, C. (2021). Modern Petrochemical Technology: Methods, Manufacturing and Applications. John Wiley & Sons.

Course Title: Advanced Instrumental Methods		I	Т	P	Cr
Paper Code: CAC.577	3	(4)	0	0	3

Total Lectures: 45

Learning Outcomes: The student will be able to

- Understand the current trends in the analysis prescribed by regulatory agencies
- Analyze the quantitative data on proteomics and metabolomics using advanced mass spectroscopy.
- Interpret and analyze the electrochemical and spectroscopic analysis set up requirement and information gathered.
- Justify use of a particular characterization technique of colloids, nanomaterial and analytes in solution.

Unit 1 11 Hours

Regulatory requirements of Food and Drug Administration (FDA) for food and drug analysis, Environmental Protection Agencies for air water and soil analysis and NABL. Uncertainty calculations and quality assurance.

Unit 2 11 Hours

Advanced Spectroscopic Analysis.: UV-Vis-NIR and its applications, Confocal Raman Spectroscopy, Time Resolved Fluorescence and Fluorescence Correlation Spectroscopic Techniques and their application, Brainstorming the application of fluorescence in quantitative information of biochemical processes.

Unit 3 11 Hours

Amperometry/Coulometry: Basic principles, constant current and constant potential coulometry. coulometric titrations.

Voltammetry: Principles, voltammograms, equation of voltammogram, different waveforms-linear scan, square scan and triangular scan, cyclic voltammetry.

Electron Microscopy including TEM, STEM, FESEM with dark field and bright field imaging.

Demonstration of electroanalytical techniques in quantitative analysis.

Peer learning activity on TEM based structural analysis of nanomaterials and thin films, electrochemical methods of analysis

Unit 4 12 Hours

Chromatographic Techniques: HRMS and MS/MS techniques for analysis of Pesticide residue, Proteomic and Metabolomic analysis. Capillary Electrophoresis.

Advanced Mass Spectroscopy: Ion cyclotron mass spectrometer, Ion Trap Mass Spectrometer, C-Trap and Orbitrap Mass spectrometry.

Team problem solving task on identification of protein using LC-HRMS data.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial **Suggested Readings:**

- 1. Tao, W. A. and Zhang, Y., (2019) Mass Spectrometry-Based Chemical Proteomics, Wiley Publishing.
- 2. Issaq, H. J. (2020) Proteomic and Metabolomic Approaches to Biomarker Discovery, Elsevier Science Publishing.
- 3. Imai, K., Yau, S. L. F., (2013) Quantitative Proteome Analysis: Methods and Applications, Jenny Stanford Publishing.
- 4. Mirzaei, H., and Carrasco, M., (2016) Modern Proteomics Sample Preparation, Analysis and Practical Applications, Springer Publishing.
- 5. Markus Sauer, M., Hofkens, J., Enderlein, J. (2010) Handbook of Fluorescence Spectroscopy and Imaging: From Ensemble to Single Molecules, Wiley Publishing.
- 6. Jameson, D. M. (2014) Introduction to Fluorescence, CRC Press.
- 7. Paul M. W. French, P. M. W., and Elson, D. S. (2014) Fluorescence Lifetime Spectroscopy and Imaging: Principles and Applications in Biomedical Diagnostics, CRC Press.
- 8. Anton Nikiforov, Nikolay Britun (2018) Photon Counting: Fundamentals and Applications, Intech Open Publishing.
- 9. Skoog, D. A., West, D. M., Holler, F. J., and Crouch, S. (2019). *Fundamentals of Analytical Chemistry*. Nelson Education.
- 10. Rouessac, F., and Rouessac, A. (2013). *Chemical Analysis: Modern Instrumentation Methods and Techniques*. John Wiley and Sons.
- 11. Gross, J. H. (2006). *Mass Spectrometry: A Textbook*. Springer Science and Business Media.
- 12. Pavia, D. L., Lampman, G. M., Kriz, G. S., and Vyvyan, J. A. (2008). *Introduction to Spectroscopy*. Cengage Learning.
- 13. Hollas, J. M. (2004). *Modern Spectroscopy*. John Wiley and Sons.
- 14. Lakowicz, J. R. (2006). *Principles of Fluorescence Spectroscopy*. Springer.

Course Title: Applied Material Chemistry	L	Т	P	Cr
Paper Code: CAC.581	3	0	0	3

Total Contact Hours: 45

Learning Outcome: The students will able to learn

- Inorganic, organic and mixed materials
- Characterization of these materials
- The relationship between material structure and physical attributes associated with them.
- Interpret and apply the conductivity of ionic and molecular conductors
- Interpret and analyse the use of materials for NLO, electronics, biomedical and energy applications

Unit 1 11 Hours

Magnetic Materials (Ferrites) Introduction, structure and classification, hard and soft ferrites, synthesis of ferrites by various methods (precursor and combustion method), characterization of ferrites by Mossbauer spectroscopy, significance of hysteresis loop and saturation magnetization in ferrites, magnetic properties of ferrites, applications of ferrites.

Glasses, Ceramics, Composites and Nanomaterials: Glassy state, glass formers and glass modifiers, applications. ceramic structures, mechanical properties, clay products. microscopic composites; dispersion–strengthened and particle–reinforced, fibre–reinforced composites, macroscopic composites, nanocrystalline phase, preparation procedures, special properties, applications.

Learning through spherical three dimensional models based demonstration and reconstruction of the models for ferrites.

Unit 2

11Hours

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic – nematic transition and clearing temperature –homeotropic, planar and sCHMieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. dielectric susceptibility and dielectric constants. lyotropic phases and their description of ordering in liquid crystals.

Thin Films and Langmuir-Blodgett Films

Preparation techniques; evaporation/sputtering, chemical process, sol gel etc. Langmuir – Blodgett (LB) films, growth technique, photolithography, properties and applications of thin and LB films

Materials for Solid State Devices

Rectifiers, transistors, capacitors –IV-V compounds, low-dimensional quantum structure; optical properties.

Application of Langmuir-Blodgett Films and materials for solid state electronics through peer learning. Brainstorming the liquid crystals based electronics and its current applications.

Unit 3 11Hours

Types of ionic conductors, Schottky and Frenkel Defects; Kronig-Vink Representation, thermodynamic characteristics, effect of doping on ionic conduction. Mechanism of ionic conduction, interstitial jumps (Frenkel) and vacancy mechanism with thermodynamic and geometric consideration. Superionic conductors including beta-alumina, NASCION, LISCION; phase transitions and mechanism of conduction in superionic conductors, applications of ionic conductors in fuel cell, batteries/cell, oxygen sensing. **Molecular Conductor:** TCNQ-TTF organic conductor, Peierls Theorem, Polyacetylene, Polyphenylene, Polyaniline, Oligo(phenylenevinylene)s, oligo(phenyleneethynylene)s, oligo(thiophenevinylene), oligo(thiophene), polypyyrole, etc. and their applications in sensing, batteries/cell,

Understanding ionic/molecular conductors and their conduction mechanism through model construction.

photovoltaic cell, actuators, biomedical application.

Unit 4 Hours

Fullerenes, Carbon Nanotubes and Graphene: Types and Properties, methods of preparation and separation of carbon nanotubes, applications of fullerenes, CNTs and graphene.

Nonlinear optical materials: Non-linear optical effects, second and third order — molecular hyperpolarisability and second order electric susceptibility — materials for second and third harmonic generation.

Preparation and characterization of silica and zirconia based stationary phases: Preparation by (a) dynamic chemical modification, in which chiral selector is adsorbed on the surface of the zirconia by physical forces, (b) permanent chemical modification, in which a CS is chemically bonded onto the zirconia surface, and (c)

physical screening. Difference between zirconia and silica based stationary phases, and their application in separations by Liquid Chromatography.

Understanding the geometry of the carbon allotropes using models.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

Suggested Readings

- 1. West, A. R. (2014). Solid State Chemistry and its Applications. John Wiley & Sons.
- 2. Smart, L. E., and Moore, E. A. (2012). Solid State Chemistry: An Introduction. CRC press.
- 3. Callister Jr, W. D., and Rethwisch, D. G. (2012). Fundamentals of Materials Science and Engineering: An Integrated Approach. John Wiley and Sons.
- 4. Anderson, J. C., Leaver, K. D., Rawlings, R. D., and Leevers, P. S. (2004). *Materials Science for Engineers*. CRC Press.
- 5. Ashcroft, N. W., and Mermin, N. D. (1976). *Introduction to Solid State Physics*. Saunders.
- 6. Keer, H. V. (1993). Principles of the Solid State. New Age International.
- 7. Dresselhaus, M. S., Dresselhaus, G., and Eklund, P. C. (1996). *Science of Fullerenes and Carbon Nanotubes: Their Properties and Applications.* Elsevier.
- 8. Rao, C. N. R., and Gopalakrishnan, J. (1997). New Directions in Solid State Chemistry. Cambridge University Press.
- 9. del Alamo, J. (2007) https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-720j-integrated-microelectronic-devices-spring-2007/
- 10. Kimerling, L.C., Saini, S. (2006) https://ocw.mit.edu/courses/materials-science-and-engineering/3-46-photonic-materials-and-devices-spring-2006/index.htm.

L	Т	P	Cr
3	0	0	3

Course Code: FST.506

Course Title: Food Chemistry

Total Hours - 45

Learning Outcome:

The completion of this course will enable learners to:

- · Explain physicochemical properties of major and minor components of foods.
- · Apply correct methods for estimating the moisture content of different foods.
- · Critically analyse chemical and nutritional properties of carbohydrates, proteins and lipids.
- Give recommendations on sources, functions, stability and requirements of vitamins and minerals.
- · Critically evaluate the effect of processing on the properties of macro components of foods.

Unit I 11 Hours

Water: Function; Types; Methods for measurement of total and available water in foods.

Carbohydrates: Classification; Occurrence; Properties and application of important polysaccharides such as starch, cellulose, guar gum, xanthan gum, pectin, etc.; Cellulose and derivatives (MCC, CMC, MC and HPMC); Starch digestibility and Glycaemic Index

Unit II 11 Hours

Proteins: Classification; Physicochemical properties of proteins; Protein structure; Forces involved in stability of protein structure; Denaturation; Functional properties; Methods of protein analysis; Protein quality and its evaluation

Unit III 11 Hours

Lipids: Classification; Functions of lipids (fat/oils) in foods; Flavour defects in lipids; Role of fats in human nutrition; Health problems associated with fats; Trans fats; Recommendations for fat intake; Non-food applications of oils and fats

Unit IV 12 Hours

Vitamins and minerals: Sources, requirements, functions stability and toxicity of vitamins; General functions of minerals; Specific functions and requirements of Ca, P, Mg, Fe, Cu, Zn, Se, etc.

Colour of foods: Chlorophylls, curcumin, betalains, carotenoids, phenolic pigments etc.; Enzymatic and Non-enzymatic browning in foods.

Transactional Modes: Lecture, presentation, Dialogue, google forms/docs, Lecture-cum-demonstration, Seminar, discussion, e-content, etc.

Suggested readings

- FA Aladedunye and R Przybylski, Degradation and nutritional quality changes of oil during frying. Journal of the American Oil Chemists' Society, 86, 149–156 (2009).
- FSSAI, Manuals published by Food Safety and Standard Authority, GOI (2016)
- HK Chopra and PS Penesar, Food Chemistry. Narosa Publication (2010).
- J Cmolíka and J Pokorny, Physical refining of edible oils. European Journal of Lipid Science and Technology,102, 472-486 (2000)
- J Hettiarachchy, Food Proteins and Peptides. CRC Press (2012)
- J Velisek, The Chemistry of Food. Wiley Blackwell (2014)
- K Owusu, Introduction to Food Chemistry. CRC Press (2015).
- MM Chakraborty, Chemistry and Technology of Oils and Fats. Prentice Hall (2003).
- P Cheung, Handbook of Food Chemistry. Springer Science (2015).
- S Bemiller, Carbohydrate Chemistry for Food Scientists, Woodhead Publications (2019).
- S Damodaran and KL Parkin, Fennema's Food Chemistry. CRC Press (2017).
- S Kumari, Basics of Food Biochemistry and Microbiology. Koros Press (2012).
- SCM Teresa, Starches for Food Application: Chemical Technological and Health Properties, Academic Press (2019).
- TAM Msagati, Chemistry of Food Additives and Preservatives. John Wiley and Sons (2013).
- Z Ustunol, Applied Food Protein Chemistry. John Wiley and Sons (2015).

L	Т	P	Cr
3	0	0	3

Course Code: BCH.509

Course Title: Bioanalytical Techniques

Total Hours: 45

Learning outcomes: Students will be able to

- Demonstrate the utility of bioanalytical techniques.
- Apply the knowledge gained in this course to understand advanced concepts of biochemistry.
- Apply and effectively communicate scientific reasoning and data analysis in both written and oral forums related to bioanalytical techniques.

Unit I 12 Hours

Spectrophotometry, Centrifugation and Biophysical Techniques: Beer-Lambert's law, extinction coefficient and its importance, design of colorimeter, spectrometer and spectrophotometer. Visible and UV Spectroscopy and its applications; Sedimentation velocity and RCF, differential and density gradient centrifugation, subcellular fractionation, analytical and preparative ultracentrifugation techniques. Optical rotatory dispersion (ORD), Circular Dichroism (CD), X-ray diffraction, X-ray absorption, Nuclear magnetic resonance spectroscopy. Seminars on application of the techniques in bioscience research.

Unit II

10 Hours

Gel Electrophoresis: Agarose gel electrophoresis for DNA and RNA analysis; Rocket electrophoresis; Polyacrylamide gel electrophoresis for DNA and protein analysis; IEF and SDS-PAGE.

Chromatography: Principles and applications of different types of chromatography. Thin layer, ion-exchange, hydrophobic-interaction, size-exclusion, Adsorption, Partition, Ion-Exchange, Chromatofocusing, Reverse Phase, and affinity chromatography. Molecular weight determination of macromolecules (in particular proteins) by size exclusion chromatography. High performance liquid chromatography.

Group discussion on the importance of gel electrophoresis and chromatography in biochemistry lab.

Unit III

12 Hours

Microscopy: Principles and applications of Light, Phase-contrast and Electron- Microscopy, Scanning electron microscope, Transmission electron microscope and Immune electron microscopy.

Radioisotopic Tracer Techniques: Detection and measurement of isotopes, Geiger–Müller, Scintillation Counter, Autoradiography, Fluorography,

Applications in biology. Student seminars on application of the techniques in research and life.

Unit IV

11 Hours

Immunological Techniques: Measurement and Characterization of antigens and antibodies, Specificity and Cross reactivity, Precipitation and Agglutination reactions, Gel Diffusion, Immunoelectrophoresis, Ouchterlony, Radioimmunoassay, ELISA, Immunoblotting, Immunoprecipitation and co-immunoprecipitation, Application in Microscopy, Imaging-Immunohistochemistry and Flow cytometry. Peer group discussion on use of the immune-techniques in research and health care.

Suggested Readings:

- 1. Berg, J.M., Stryer, L., Tymoczko, J., Gatto, G. (2019). Biochemistry. WH Freeman. 9th ed.
- 2. Nelson DL, Cox MM and A. Hoskins (2021). Lehninger's Principles of Biochemistry, 8th ed. WH Freeman.
- 3. Wilson, K., Walker, J. (2018). Principles and Techniques of Biochemistry and Molecular Biology. 8th Edition, Andreas Hofmann and Samuel Clokie, Cambridge University Press.
- 4. Iain D Campbell (2012). Biophysical Techniques, Oxford University Press.
- 5. Shourie, A., Chapadgaonkar, S.S. (2015). Bioanalytical Techniques. TERI, New Delhi.

Web resources:

- https://www.youtube.com/watch?v=siXdckB1HzU
- https://www.youtube.com/watch?v=WP6JpnHZJIQ
- https://www.youtube.com/watch?v=pjG4FTdMsEY
- https://nptel.ac.in/courses/102/103/102103044/
- https://nptel.ac.in/courses/102/101/102101007/
- https://www.youtube.com/watch?v=yl3EZX5kKbM
- https://www.youtube.com/watch?v=yl3EZX5kKbM
- https://www.youtube.com/watch?v=eH7UkTB7m8U
- https://www.youtube.com/watch?v=vMzs4NyVvuc
- https://www.youtube.com/watch?v=ZN7euA1fS4Y

Modes of transaction

-Lecture cum Demonstration

- -Problem solving approach
- -Self Learning
- -Inquiry training
- -Team learning

Tools used

PPT, You tube Video, Google meet, NPTEL

L	Т	P	Cr
0	0	8	4

Course Title: Research Proposal

Paper Code: CAC.599 Total Contact Hours: 120

Course Outcome: The student would be able to

• Investigate various aspects related to the chemistry problem.

• Generate interest in frontier areas of research in chemistry.

• Analyze the literature and bring forward the research gaps and propose hypotheses and tentative solutions.

Dissertation supervisor would be allocated at the start of the semester and entire dissertation would be undertaken in discussion with the supervisor. At the end of the semester the student has to prepare a research proposal/synopsis as per the university guidelines. Upon submission of the synopsis, the research proposal shall be evaluated based on a presentation of review of literature, research gap, objective, methodology and PERT Chart for the next semester for sections of experimental work and compilation of dissertation.

L	Т	P	Cr
0	0	4 0	20

Course Title: Dissertation

Paper Code: CAC.600 Total Contact Hours: 600

Learning Outcome: The student would be able to

- Understand the lacunas in the methodology to experimentation.
- Independently plan and execute experiments in the laboratory set-

up

- Analyze and interpret the results obtained through different experiments.
- Apply their expertise and specific skills in the frontier area of research.

As per the defined objectives in the research proposal/synopsis, the student would carry out his experimentation to achieve these goals. The student would get experiments evaluated by the supervisor regularly, wherein the progress of the student would be evaluated. Upon achieving the objectives of the synopsis, the dissertation would be prepared as per the university guidelines for M.Sc. Dissertation in consultation with the supervisor. Dissertation would be verified for plagiarism and submitted for evaluation by committee.

Interdisciplinary Courses (IDCs)

L	Т	P	Cr
2	0	0	2

Course Title: Introduction to Green Chemistry and Sustainability

Paper Code: CHM.516 Total Contact Hours: 30

Learning objective: Students will be able to

• Know the concept and various tools of Green Chemistry.

- Explain the relevance of Green Chemistry in the context of environment issues.
- Realize the judicious utilization of abundantly available precursors instead of depleting petroleum based feedstocks.

Unit 1 Tours

Introduction: Adverse effect of some of the current chemical practices on health and environment, concept and need of green chemistry, basic principles of green chemistry with examples— atom economy, wastage minimization, selection of starting materials etc. limitations/obstacle in the persuit of the goals of green chemistry, types of solvent.

Relevance of the various principles of Green chemistry in various areas for sustainable development through brainstorming.

Unit 2 Hours

Emerging non-conventional techniques: Microwave heating as energy efficient source, mechanism of microwave heating, Examples of microwave assisted organic synthesis, sono-chemistry and green chemistry.

Various emerging energy efficient tools and their heating mechanism for conducting chemical reactions through collaborative approach.

Unit 3

Hours

Green solvents: Ionic liquids: properties and advantages, use of ionic liquids as solvent as well as catalyst, recyclability of ionic liquids. Solvent-free synthesis.

Recyclability of ionic liquids through demonstration and discussion on their potential use as a replacement for halogenated volatile organic. solvents.

Unit 4 8 Hours

Value addition of abundantly available precursors: Need for the use of renewable precursors over petroleum based feedstocks, biomass conversion (carbohydrates, lignocellulose biomass) into value added molecules.

Progress and challenges for the conversion of biomass into value added chemicals through peer group learning.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

Suggested Readings

- 1. Ahluwalia, V.K and Kidwai, M. (2012) New Trends in Green Chemistry. Springer.
- 2. Anastas, P.T. and Warner J. C. (2000) *Green chemistry: Theory and Practical*. Oxford University Press, US.
- 3. Malhotra, S. V. (2007) *Ionic Liquids in Organic Synthesis*. Oxford University Press, US.
- 4. Ahluwalia, V.K. (2011) Green Chemistry: Greener Alternatives to Synthetic Organic Transformations. Alpha Science International Limited.
- 5. Gaudino, E. C., Cravotto, G., Manzoli, M., & Tabasso, S. (2019). From waste biomass to chemicals and energy via microwave-assisted processes. *Green Chemistry*, 21(6), 1202–1235.
- 6. Clauser, N. M., González, G., Mendieta, C. M., Kruyeniski, J., Area, M. C., & Vallejos, M. E. (2021). Biomass waste as sustainable raw material for energy and fuels. *Sustainability*, 13(2), 794.

L	T	P	Cr
2	0	0	2

Course Title: Chemistry of Nanomaterials and Fabrication

Paper Code: CHM.517 Total Contact Hours: 30

Learning Outcome: The students will acquire knowledge of Nanotechnology, fabrication and characterization of nanomaterials, properties and applications of nanomaterials.

Unit 1 7Hours Background to Nanotechnology:

Scientific revolution - Atomic structures - molecular and atomic size - Bohr radius - emergence of nanotechnology - challenges in nanotechnology. Definition of a nano system - types of nanocrystals - one dimensional (1D) - two dimensional (2D) - three dimensional (3D) nanostructured materials - quantum dots - quantum wire - multifunctional nanostructures.

Relevance of the various aspects of Nano chemistry in various areas for sustainable development through brainstorming.

Unit 2 Hours

Fabrication and Characterization of Nanomaterials: Top-down and bottom-up approaches: chemical routes for synthesis of nanomaterials: chemical precipitation and co-precipitation; metal nanocrystals by reduction, sol-gel synthesis; microemulsions or reverse micelles, myle formation; solvothermal synthesis; thermolysis routes, microwave heating synthesis; sonochemical synthesis; electrochemical synthesis. physical methods: -inert gas condensation, arc discharge, plasma arc technique, MW plasma, laser pyrolysis, molecular beam epitaxy, chemical vapour deposition method and electro deposition. diffraction analyses, imaging techniques, spectroscopic techniques.

Various advanced techniques for nanomaterials characterization and their formation mechanism through collaborative approach.

Unit3 8 Hours

Nanomaterials and properties: Influence of nucleation rate on the size of the crystals – macroscopic to microscopic crystals and nanocrystals – large surface to volume ratio. Metals (Au, Ag) – metal oxides (TiO2, CeO2, ZnO etc.) – semiconductors (Si, Ge, CdS, ZnSe) – carbon nanotubes (CNT) – ceramics and composites – dilute magnetic semiconductor – biological system – DNA and RNA – lipids – size dependent properties – mechanical, physical and chemical properties.

Concept of Nano dimension materials fabrication.

Unit 4 Hours

Applications of Nanomaterials: Photocatalysis – solar cell-water splitting-energy harvesting – LSPR – molecular electronics and nanoelectronics-quantum electronic devices – CNT based transistor and field emission display –biological applications – biochemical sensor – MRI agent – nanomedicine: molecular manufacturing – MEMS – NEMS – Bio – MEMS – protein nanoarrays – nano fluidics and micro fluidics – self – assembly of nanoparticles for biomedical applications – bacterial structures – cubosomes – dendrimers – DNA nanoparticle conjugates – bioactive nanomaterials – Au nanoparticles and CdSe quantum dots – molecular motors – nanoparticle and protein interactions.

Concept of Nano dimension materials for modern applications.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming.

Suggested Readings

- 1. Rao, C. N. R., Müller, A. and Cheetham, A. K. (Eds.) (2004). The Chemistry of Nanomaterials: Synthesis, Properties and Applications. Willy-VCH.
- 2. Poole, Jr., C. P. and Owens F. J. (2006). Introduction to Nanotechnology, Willy-VCH
- 3. Mukhopadhyay, S. M., (2012) Nanoscale Multifunctional Materials: Science and Applications. Willy-VCH
- 4. Kelsall, R. W., Hamley, I. W. and Geoghegan, M. (2005). *Nanoscale Science and Technology*. 2005, John Wiley and Sons.

L	T	P	Cr
2	0	0	2

Course Title: Basic Perspectives in Inorganic Chemistry

Paper Code: CHM.515 Total Contact Hours: 30

Learning Outcome: The student will able to

- Become expertise of the coordination chemistry of d-group elements and coordination of ions within living organisms.
- Know the environmental chemistry and metal hydrides as hydrogen energy source.

Unit 1 7Hours

Chemistry of d-block elements. coordination chemistry, models and stereochemistry, theories, spectra and bonding.

Group discussion and problem solve involving characteristics of transition metals and their compounds.

Unit 2

8Hours

Ions role in bioscience: ionophores, porphyrin and other tetrapyrrollic macromolecules, coenzymes, neurotransmitters, metal binding to DNA.

Brainstorming discussion about essential inorganic elements and their compounds in living organisms

Unit 3 8Hours

Metals in aqueous environment: Introduction, environmental chemistry, environmental composition, chemical processes, complexes, metal speciation of calcium, copper and mercury, their behaviour in hydrosphere.

Discussion on behaviour of metals and complexes in surrounding environmental sphere

Unit 4

7Hours

Hydrogen Energy: introduction, synthesis and structures of metal hydrides, coordination modes of hydrogen atom, hydrogen storage, H₂ evolution under solar energy, thermal energy and acidifications.

Group discussion about current requirements and challenges of renewable energy resources.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

Suggested Readings

- 1. Lippard, S.J. and Berg, J.M., (1994) *Principles of Bioinorganic Chemistry*. University Science Books.
- 2. Cotton, F. A., and Wilkinson, G. (1988). Advanced Inorganic Chemistry (Vol. 545). New York: Wiley.
- 3. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
- 4. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
- 5. Van-Loon G.W. and Duffy S.J. (2011) Environmental Chemistry: A Global Perspective. Oxford University Press.
- 6. Rao C.S. (2006) *Environmental Pollution Control Engineering*. New Age International Publishers, New Delhi,
- 7. Peruzzini, M. and Poli, R. (2005) *Recent Advances in Hydride Chemistry*, Elsevier Science B.V., Amsterdam.

Course Title: Chemicals of Everyday life		L	Т	P	Cr
Paper Code: CHM 519		2	0	0	2

Total Lectures: 30

Learning objective: Students will be able to

- Know the utility of various chemical in daily life.
- Explain the importance of green approaches as the need of the hour

Unit 1 7

Hrs

Chemicals and safety

Chemicals in daily life, Cosmetics, Perfumes, Soaps and detergents, Cleaning action of detergent, Handling of strong acids and bases, Disinfectant, Insecticides and pesticides, Chemical treatment of vegetables and fruits

Project work on list of chemicals used in the kitchen and in personal hygiene Project work on chemical constituents present in various spices used in the kitchen, fruits and vegetables

Unit 2
Hrs

Common chemical processes

Chemical reactions, Basics of organic synthesis, Chemistry of photosynthesis, Rusting, Electrochemical cells, Metal electroplating, Acid base titration in the lab

Use of polymers in daily life, Polymer based products, Teflon, Polystyrene, Plastic bags, ATM cards.

Discussion on chemical composition of daily use articles like soap, shampoo, toothpaste etc.

Unit 3
Hrs

Chemistry of small bioactive molecules

Caffeine, Nicotine, Paracetamol, Aspirin, DNA and RNA bases, Carbohydrates

Abused substances like morphine, Cannabis, Cocaine etc.

Use and overuse of medicines: a debate

Unit 4
Hrs

Green chemical processes

Environment friendly process, Principle of green chemistry, Atom economy and scope, Prevention/Minimization of hazardous/toxic products, designing safer chemicals, Selection of appropriate auxiliary substances (solvents, separation agents etc.), Use of renewable starting materials, Avoidance of unnecessary derivatization–careful use of blocking/protection groups

Microwave in organic synthesis: Introduction to synthetic organic transformation under microwave (i) Microwave assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave in solvent free reactions.

Sustainable lifestyle: peer discussion in the classroom

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial.

Suggested Readings

- 1. Singh, K.; Chemistry in Daily Life, PHI learning, 3rd edition India
- 2. Glasstone, S.; Chemistry in Daily Life, Cornell University, Methuen & Company Limited, 1929
- 3. Cohan, L.; Chemistry in Daily Life; Popular Lectures, HardPress, 2012
- 4. Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical.* Oxford University Press, 1st edition, US.
- **5.** Grieco, P.A. (1997). *Organic Synthesis in Water*. Blackie, 1st edition

L	Т	P	Cr
2	0	0	2

Course Title: General Laboratory Practice

Paper Code: CHM.518 Total Contact Hours: 30

Learning Outcome: The students will acquire knowledge of

- Good laboratory practices
- Quality control and Quality assurance
- Chemical, biological and radiation hazards in laboratory and safety.
- General know how of analytical sample preparation.

Unit 1 7 Hours

Good Laboratory Practices: Introduction and WHO guidelines on GLP and GMP. History of GLP. Quality assurance in GLP. Quality control laboratory, responsibilities, routine controls, instruments reagents, sampling plans. Regulatory requirement through gaming a laboratory for GLP through dramatization.

Unit 2 8 Hours

Quality Standards and Quality Assurances: Advantages and disadvantages of quality standards, concepts of quality control, quality assurance its functions

and advantages. Standard test procedures, protocols, non-clinical testing, controls on animal house, data generation and storage, quality control documentation, retention samples, records. Complaints and recalls, evaluation of complaints, recall procedures, related records and documents.

Understanding the quality deliverability of disciplinary laboratory through team brainstorming.

Unit 3 8 Hours

Safety and Hazard Analysis: Chemical classification of hazards, Radiation hazard, AERB regulation for Fire and its prevention, biosafety and biohazard. Weapons of Mass destruction

Understanding National and international regulatory requirements of chemical and bio-hazards through hands-on inspection of laboratory.

Unit 4 Hours

Basic Analytical practices: Titrimetry, Gravimetric analysis, Potentiometry and Spectrophotometric analysis. Pesticides and pesticide residue extraction, Solid phase extraction etc. Trace metal sample preparations and analysis. Proteomic and metabolomic sample preparations

Understanding the selection of analytical procedures for analysis and sample preparation methods using peer learning.

- 1. Miller, J. C. and Miller, J. N. (1998) Statistics for Analytical Chemistry. Wiley.
- 2. Skoog D. A., Holler, F. J., Crouch, S. R. (2018) Principles of Instrumental analysis Cengage Learning
- 3. Holler, F. J., Crouch, S. R., West, D. M., and Skoog D. A.,(2014) Fundamental of Analytical Chemistry, 9th ed. Cengage Learning http://www.who.int/water_sanitation_health/resourcesquality/wq mchap9.pdf
- 4. https://www.unece.org/fileadmin/DAM/env/water/publications/doc uments/guidancela boratories.pdf.
- 5. https://www.ugc.ac.in/oldpdf/xiplanpdf/disposalofradioactiv.pdf
- 6. https://www.mea.gov.in/Uploads/PublicationDocs/148_The-Weapons-Mass-destruction-And-Delivery-Systems-Act-2005.pdf
- 7. Westgard, J. O., Barry, P. L. (2016) Basic QC Practices: Training in Statistical Quality Control for Medical Laboratories, 4th ed., Westgard Quality Corporation.
- 8. Kenkel, J. (2014) Analytical Chemistry for Technicians, 4th ed., CRC Press.

- 9. Konieczka, P., Namiesnik, J., (2018) Quality Assurance and Quality Control in the Analytical Chemical Laboratory: A Practical Approach, 2nd ed. CRC Press.
- 10. WHO (2011) Laboratory Quality Management System Handbook.
- 11. Zaman, G., (2018) Quality Control in Laboratory, Intech Open Publishing.
- 12. Hasnain, M.S., Beg, S., (2019) Pharmaceutical Quality by Design: Principles and Applications, Elsevier Science.

L	Т	P	Cr
2	0	0	2

Course Title: Chemistry of Drug Design and Synthesis

Paper Code: CHM 520 Total Contact Hours: 30

Learning Outcome: At the end of this course student will be able to

- Rationalize the basis of drug design, drug action and drug metabolism.
- Apply the knowledge to design and synthesize different drug molecules.
- Interpret the mechanism of action of different classes of drugs.

Unit 1 8
Hrs

Basics of Drug Action

Weak interactions in drug molecules, Covalent, ion, ion-dipole, hydrogen bonding and van der Waals interactions, Drug-receptor interactions, receptor theories and drug action, Occupancy theory, rate theory, induced fit theory, macromolecular perturbation theory, activation-aggregation theory, enzyme kinetics in drug action, mechanisms of enzyme catalysis.

Apply the knowledge of drug-receptor interactions in drug design through peer learning

Unit 2
Hrs

Drug Design

Introduction, Structure Activity Relationships in drug design: Qualitative versus quantitative approaches, advantages and disadvantages; rational approaches to lead discovery, bioisosterism, Insights into molecular

recognition phenomenon; Structure based drug design, ligand based drug design.

Class discussion of molecular modelling in structure based and ligand based drug design approach

Unit 3
Hrs

Drug Metabolism

Biotransformation of drugs, enzymes responsible for bio-transformations, microsomal and non-microsomal mechanisms; Factors influencing enzyme induction and inhibition, Factors effecting drug metabolism; Models to study drug metabolism, Adverse drug reactions; toxic reactions, allergic reactions.

Usefulness of different models to study drug metabolism through peer discussion

Unit 4

8 Hrs

Mechanism of action and synthesis of various drugs

Introduction to parasitic and infectious diseases, Mechanism of action of anti-tuberculosis drugs, anti-HIV drugs, anti-malarial drugs, anti-leishmanial drugs and anti-cancer drugs. Mechanism of drug resistance in infectious disease. Synthesis of anti-tuberculosis, anti-HIV, anti-malarial, anti-leishmanial and anti-cancer drugs.

Recent advances on anticancer and antibiotic drug synthesis through brainstorming

- 1. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*. 4th Edition, Oxford University Press.
- 2. Coulson, C.J. (1994). *Molecular Mechanisms of Drug Action*, 2nd Edition, Taylor & Francis, London.
- 3. Silverman, R.B., Holladay, M.W. (2014). *The Organic Chemistry of Drug Design and Drug Action*, 3rd Edition, Academic Press.
- 4. Leach, A.R. (2001). Molecular Modelling: *Principles and Applications*, Prentice Hall.
- 5. Cohen, C. (1996). *Molecular modeling in Drug Design*, Academic Press.

- 6. Gibson, G.G., Skett, P. (2013). Introduction to Drug Metabolism, 2nd edition, Springer, US.
- 7. Bancet, A., Raingeval, A., Lomberget, T., Borgne, M-L., Guichou, J-F., Krimm, I. Fragment Linking Strategies for Structure-Based Drug Design, *J. Med. Chem.* 2020, 63, 20, 11420–11435.
- 8. Flick, A. C., Leverett, C. A., Ding, H. X., McInturff, E., Fink, S. J., Mahapatra, S., Carney, D. W., Lindsey, E. A., DeForest, J. C., France, S. P., Berritt, S., Bigi-Botterill, S. V., Gibson, T. S., Liu, Y., O'Donnell, C. J. Synthetic Approaches to the New Drugs Approved during 2019, *J. Med. Chem.* 2021, 64, 7, 3604–3657.

Value Added Course (VAC)

Course Title: Protein Chemistry		Т	P	Cr
Paper Code: CHM.528		0	0	2

Total Contact Hours: 30

Learning Outcome: The students will able to interpret and analyze

- Structure and biological functions of proteins.
- The role of metals in biology
- Mechanism of protein folding
- The cause and treatment of neurodegenerative, iron metabolic disorder and diabetes.

Unit: 1 7 Hours

Buffers; Amino Acids; Proteins: Function and Structure, Protein synthesis; Protein engineering and protein/protein interactions.

Group discussion regarding in-vivo and in vitro protein folding.

Unit: 2
Hours

Structure and function of hemoglobin, myoglobin and transferrin; Iron metabolic disorders (anemia, Sickle cell anemia. thalassemia. hemochromatosis), Diabetes: of diabetes and **Types** its causes/prevention/treatment, Interlink between iron metabolic disorder and diabetes; Cancer and its causes/treatments.

Brainstorming regarding the role of metals in health and diseases and interlink between iron metabolic disorder and diabetes.

Unit: 3 8 Hours

Protein folding and misfolding, Determination of protein structures and folding intermediates; In vitro analyses of off-pathway aggregation and amyloid formation; Key chaperones and chaperonins;

Peer group discussion on understanding how protein folds/misfolds and forms amyloid fibrillation and their treatment and diagnosis.

Unit: 4. 7 Hours

Practical implications in biotechnology; Special emphasis on human protein deposition diseases including Alzheimer's, Parkinson's and Huntington's disease.

Demonstration of role of chaperones and peptides on preventing amyloid fibril formation in human natively disordered proteins.

Mode of Transactions: Demonstration, Experimentation, handing instruments, Explanation of data

- 1. Donev, R. (2021) Advances in Protein Chemistry and Structural Biology-Protein misfolding, Academic Press Inc.
- 2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). Inorganic chemistry: Principles of Structure and Reactivity. Pearson Education India.
- 3. Douglas, B. E., and McDaniel, D. H. (1965). Concepts and models of inorganic chemistry. John Wiley and Sons.
- 4. Cotton, F. A., and Wilkinson, G. (1988). Advanced inorganic chemistry (Vol. 545). New York: Wiley.
- 5. Elschenbroich, C. (2016). Organometallics. John Wiley and Sons.
- 6. Atkins, P., Overtone, T., Rourke, J., Weller, J., and Armstrong, F., (2010). Shriver and Atkins' inorganic chemistry. Oxford University Press.
- 7. Cowan, J. A. (1997). *Inorganic Biochemistry: An Introduction*. Wiley VCH.
- 8. Lippard, S. J. (1991). Progress in Inorganic Chemistry. Vol. 18, Wiley-Interscience.
- 9. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vol. 38, Wiley-Interscience.
- 10. Lesk, A. M., (2010). *Introduction to Protein Science: Architecture, Function, and Genomics*. Oxford University Press.

- 11. Cantor, C. R. and Schimmel, P. R., (1980). *Biophysical Chemistry*. Freeman.
- 12. Van Holde, K. E., Johnson, W.C., and Ho, P. S., (2006). *Principles of Physical Biochemistry*. Pearson Education.
- 13. Harding, S. E. and Chowdhry, B. Z. (2001). *Protein–Ligand Interactions*. Oxford University Press
- 14. https://sickle.bwh.harvard.edu/index.html
- 15. https://sickle.bwh.harvard.edu/iron_transport.html

Course Title: Biological Inorganic Chemistry			T	P	Cr
Paper Code: CHM.531		2	0	O	2

Total Contact Hours: 30

Learning Outcome: At the end of this course student will be able to

- Determine the structure and biological functions of enzymes and metalloproteins.
- Classify the metallobiomolecules on the basis of their functional properties.
- Ascertain the role of metal ions and non-metals in the biological system.

Unit 1 7 Hours

Co-ordination chemistry: Introduction to bioinorganic chemistry: biological roles of elements, Coordination Complexes, Characteristics of coordination compounds, Bonding in complexes, Coordination of metal ions in biological molecules. Pearson's Hard and Soft acids and bases: application to predict the stability of complexes.

Peer discussion of selection of specific metal ions by specific enzyme. Deliberation on the role of metal ions in stabilization of protein structures.

Unit 2 7 Hours

Alkali and Alkaline earth metal ions in biological systems: Regulatory role of Na⁺ and K⁺ ions. Sodium-potassium ATP-ase, Natural and synthetic ligands for alkali metal ions, Lithium as anti-mania agent, Calcium metabolism (absorption, excretion, hormonal control), The calcium signal, calcium binding proteins, role of Mg²⁺ in biological system, magnesium in cellular physiology.

Brainstorming on the role of various metal ions in the functioning of various enzymes.

Unit 3 8 Hours

Transition metal ions in biological system: Biochemistry of iron, Iron metabolism (absorption, transport, storage, hemosiderosis, hemochromatosis), Iron in hemoglobin, Heme proteins, Cytochrome P-450, Non-heme iron containing proteins. Iron-sulfur clusters, iron storage and transport, ferritin, transferrin. Iron overload disorder. Role of Cu in biological systems (Ceruloplasmin, Cytochrome c oxidase, Cu-Zn-superoxide dismutase, Tyrosinase), Wilson's disease, Menkes disease. Role of Mn, Ni, Mo, Co and Zn (Zn-finger proteins,) in the biological system. Role of toxic metals like Pb, Hg and Cd in the biological system. Chelation therapy and application of Deferasirox, DMSA. Application of cis-platin and Myocrisin.

Group discussion on the role of metal ions in various disease conditions and chelation therapy.

Unit 4 8 Hours

Inorganic chemistry of enzymes: Metalloporphyrins: Hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, Bohr effect, structure and function of hemoglobin and myoglobin. Other iron-porphyrin biomolecules, peroxidases and catalases, cytochromes, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer. Metallothioneins: Ferredoxins, carboxypeptidase, carbonic anhydrase, blue copper proteins, superoxide dismutase and hemocyanins.

Group discussion on artificial Iron-sulfur clusters.

Mode of Transactions: Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brainstorming, Tutorial

- 1. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic chemistry: principles of structure and reactivity.* Pearson Education India.
- 2. Douglas, B. E., and McDaniel, D. H. (1965). Concepts and models of inorganic chemistry. John Wiley and Sons.
- 3. Cotton, F. A., and Wilkinson, G. (1988). *Advanced inorganic chemistry* (Vol. 545). New York: Wiley.
- 4. Elschenbroich, C. (2016). Organometallics. John Wiley and Sons.
- 5. Atkins, P., Overtone, T., Rourke, J., Weller, J., and Armstrong, F.,(2010). Shriver and Atkins' inorganic chemistry. Oxford University Press.
- 6. Cowan, J.A. (1997). *Inorganic Biochemistry: An Introduction*. Wiley VCH
- 7. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vol. 18, Wiley-Interscience.

- 8. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vols. 38, Wiley–Interscience.
- 9. Lesk, A.M., (2010). Introduction to Protein Science: Architecture, Function, and Genomics. Oxford University Press.
- 10. Cantor, C.R. and Schimmel, P.R., (1980). *Biophysical Chemistry*.Freeman.
- 11. Van Holde, K.E., Johnson, W.C., and Ho, P.S., (2006). *Principles of Physical Biochemistry*. Pearson Education.
- 12. Harding, S.E. and Chowdhry, B. Z. (2001). *Protein–Ligand Interactions*. Oxford University Press.
- 13. Kepp, K. P., Bioinorganic Chemistry of Alzheimer's Disease. Chemical Reviews 2012, 112, 10, 5193–5239.
- 14. Snyder, B. E. R., Bols, M. L., Schoonheydt, R. A., Sels, B. F. and Solomon, E. I. Iron and Copper Active Sites in Zeolites and Their Correlation to Metalloenzymes. Chemical Reviews 2018, 118, 2718–2768.
- 15. Huang, X., and Groves, J. T., Oxygen Activation and Radical Transformations in Heme Proteins and Metalloporphyrins. Chemical Reviews, 2018, 118, 2491-2553.

т	Т	D	С
ь	_	P	r
2	0	0	2

Course Title: Spectroscopic and Chromatographic Techniques

Paper Code: CHM.532 Total Contact Hours: 30

Learning Outcome: At the end of this course student will be able to

- Explain the principle and instrumentation associated with various spectroscopic techniques.
- Identify various spectroscopic techniques and their use in various streams for structure identification.

Unit 1 6 Hours

UV-Visible spectroscopy: Electromagnetic spectrum. Interaction of electromagnetic radiation with matter and various transitions giving rise to ultraviolet and visible spectra. Intensity of bands. Instrumentation, theory and principle, how to run and analyze UV-Vis spectra.

Infrared Spectroscopy: Theory and Instrumentation, Infrared radiation and its interaction with organic molecules, vibrational mode of bonds, Preparation of Samples for Infrared Spectroscopy, interpretation of IR spectra.

Role of UV-Vis and IR techniques in research and industry through peer learning

Unit 2 8 Hours

Mass spectrometry: Basic principle and brief outline of instrumentation.

Application of Mass Spectroscopy in Pharmaceutical, agricultural practices metabolomics, geoscience, food and nutrition domains.

Ion formation techniques: EI, CI, FAB, MALDI, fragmentation process of molecules. High resolution mass spectrometry (HRMS).

Inductively coupled plasma mass spectrometry (ICP-MS) and Atomic absorption spectroscopy (AAS): overview of these techniques for the determination of trace metals.

Identification and interpretation of various peaks in the mass spectrum through demonstration.

Comparison of AAS and ICP-MS techniques for determination of heavy metals through group presentation.

Unit 3 Hours

Nuclear magnetic resonance spectroscopy (NMR): Basic principle of NMR and instrumentation. chemical shift (shielding of the nuclei by the local electronic structure) and factors influencing chemical shift, reference standards and NMR solvents. spin-spin coupling, coupling constants.

¹³C NMR Spectroscopy.

Interpretation of various peaks for structural identification through demonstration of various ¹H and ¹³C NMR spectrum.

Unit 4 6 Hours

Chromatographic Techniques

Principles and Fundamentals of chromatography, Thin Layer chromatography, Column liquid chromatography.

HPLC: Applications of HPLC for identification, quantification and purification of the individual components of the mixture, HPTLC, Ion exchange chromatography.

Latest research on the utility of HPLC and UPLC in pharmaceutical analysis of drugs through group presentation.

Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

- 1. Pavia, D. L., Lampman, G. M., Kriz, G. S., and Vyvyan, J. A. (2015). *Introduction to Spectroscopy*. Cengage Learning India Private Limited; 5th edition (14 January 2015).
- 2. Gross, J. H. (2017). *Mass Spectrometry: A Textbook*. Springer-Verlag Berlin Heidelberg.

- 3. Kalsi, P. S. (2016). *Spectroscopy of Organic Compounds*. New Age International.
- 4. Kemp, W. (2019, 2nd edition). Organic Spectroscopy, ELBS. MACMILLAN
- 5. Melinda, J.D. (2010). *Introduction to Solid NMR Spectroscopy*. Wiley India Pvt Ltd.
- 6. Silverstein, R. M., Webster, F. X., Kiemle, D. J., and Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley and sons.
- 7. Pretsch, E., Bühlmann, P., Badertscher, M. (2020). Structure Determination of Organic Compounds. Springer-Verlag Berlin Heidelberg.
- 8. Webb, G. A. (2021). Annual Reports on NMR Spectroscopy. Elsevier
- 9. Corradini, D. (Ed.). (2016). Handbook of HPLC. CRC Press.
- 10. Priyanka, G., Sravani, G., & Kranthi, A. (2020). Overview on HPLC method development and standardization for drugs. *International Research Journal of Pharmaceutical and Applied Sciences*, 10(2), 15–18.