Central University of Punjab

Course Structure and Syllabus

M.Sc. Chemistry

Session: 2021-23

Department of Chemistry
School of Basic Sciences

Graduate Attributes

The Graduates will be able to identify various aspects of chemicals and their importance in consumer products. After completing M.Sc. in Chemistry, the graduates will have comprehensive knowledge and understanding of all the domains of Chemical Sciences, for application in multidisciplinary environments including biological, chemical and physical sciences. They will have sufficient expertise in problem solving by applying critical, creative and evidence based thinking to conceive innovative responses to future challenges.

They will engage in professional behaviour and have entrepreneurial potential and will be able to take leadership roles in their occupations, careers and community with ethical behaviour. They will be able to contribute to multicultural, IT revolutionized and sustainable society/policy with the attributes of global citizens. Moreover, this program will help the graduates to make their bright career in academic, research, and industry.

Semester I

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CHM.506	Fundamental Biology *	CF	2	1	0	3
	CHM.507	Fundamental Mathematics**	CF	2	1	0	
2	CHM.509	Inorganic Chemistry – I	C	3	0	0	3
3	CHM.510	Organic Chemistry – I	C	3	0	0	3
4	CHM.511	Physical Chemistry – I	C	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				**16**	**1**	**8**	**21**
Interdisciplinary Course Offered by Department for other Departments							
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	ID	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. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CHM.521	Inorganic Chemistry – II	C	3	0	0	3
2	CHM.522	Organic Chemistry – II	C	3	0	0	3
3	CHM.523	Physical Chemistry – II	C	3	0	0	3
4	CHM.524	Spectroscopic Analysis	C	3	0	0	3
5	CHM.525	Molecular Spectroscopy	C	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
Total Credit (Hours)				**18**	**0**	**8**	**22**
Value Added Course offered by Department to other Departments							
10.	CHM.528	Protein Chemistry	VAC	2	0	0	2
11.	CHM.503	Biological Inorganic Chemistry	VAC	2	0	0	2
12.	CHM.504	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	Course Type	L	T	P	Cr
1	CHM.551	Inorganic Chemistry-III	**C**	**3**	**0**	**0**	**3**
2	CHM.552	Organic Chemistry-III	**C**	**3**	**0**	**0**	**3**
3	CHM.563	Advanced Chemistry-I (Practical)	**SB**	**0**	**0**	**4**	**2**
4	CHM.559	Advanced Logics in Chemistry	**DEC**	**2**	**0**	**0**	**2**
5	CHM.600	Research Proposal	**SB**	**0**	**0**	**8**	**4**
Opt Any **Three** (**03**) Discipline Elective Courses				**9**	**0**	**0**	**9**
6	CHM.560	Solid State Chemistry	**DE**	3	0	0	3
7	CHM.561	Polymer Chemistry	**DE**	3	0	0	3
8	CHM.562	Inorganic Photochemistry	**DE**	3	0	0	3
9	CHM.576	Organotransition Metal Chemistry	**DE**	3	0	0	3
10	CHM.579	Current Trends in Organic Synthesis	**DE**	3	0	0	3
11	CHM.520	Green Chemistry	**DE**	3	0	0	3
12	CHM.574	Advanced Organic Synthesis	**DE**	3	0	0	3
13	CHM.553	Bioinorganic and Biophysical Chemistry	**DE**	3	0	0	3
14	CHM.575	Chemistry of Natural Products	**DE**	3	0	0	3
15	CHM.580	Supramolecular Chemistry	**DE**	3	0	0	3
16	CMC.510	Medicinal Chemistry-I	**DE**	3	0	0	3
17	CMC.523	Fundamentals of Computer Aided Drug Design	**DE**	3	0	0	3
18	BCH.508	Biomolecules and Bioenergetics	**DE**	3	0	0	3
Total				**17**	**0**	**12**	**23**

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

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

<u>Semester-IV</u>

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CHM.600	Dissertation	**SB**	**0**	**0**	**40**	**20**
		Total		**0**	**0**	**40**	**20**

SB: 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	
	Marks	**Evaluation Methods**	**Marks**	**Evaluation Methods**	**Marks**	**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 very short answers (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)		
	Marks	**Evaluation Method**		**Marks**	**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	50	Dissertation proposal and presentation	External expert, HoD and senior-most faculty of	50	Dissertation report (30), presentation (10), final viva-voce (10)

			the departmen t		

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	T	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	T	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

Suggested Readings

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	T	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 10 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 10 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 **10 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

Suggested Readings

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	T	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^i 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 betweenS_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, H_2O, hydride ion, ammonia derivatives, $LiAlH_4$, $NaBH_4$, 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

Suggested Readings

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	T	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 **11 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 **11 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, CO_2 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 **11 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

Suggested Readings

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	T	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 H_2^+ and H_2, Shape of molecules, Hybridization and valence MOs of H_2O and NH_3. Determination of bond angle in sp^3, sp^2 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	**T**	**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 Ba^{2+} 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 Cu^{2+}as cuprous thiocyanate.

Precipitation Titrations

1. $AgNO_3$ standardization by Mohr's method.
2. Volhard's method for Cl^- determination.

Oxidation-Reduction Titrations

1. Standardization of $KMnO_4$with sodium oxalate and determination of Ca^{2+} 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 KIO_3 titration.

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

Suggested Readings

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	T	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_f values: identification of unknown organic compounds by comparing the R_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 $NaBH_4$.
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	T	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 **10 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

Suggested Readings

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	T	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 **12 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 **11**
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

Suggested Readings

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	T	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 **11 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 **11 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. Lab-on-chip based flow cell reactors using peer learning.

Unit 4 **11 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

Suggested Readings

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.0c00837
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	T	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, ^{1}H &^{13}C 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. ^{19}F, ^{15}N, ^{31}P.

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

Unit 3
11 Hours
^{13}C NMR: Introduction, Proton coupled and proton decoupled ^{13}C NMR, nuclear overhauser enhancement (NOE), DEPT techniques, 2D NMR Correlation spectroscopy (COSY), Homo COSY (^{1}H-^{1}H COSY), Hetero COSY (^{1}H-^{13}C COSY, HMQC), long range ^{1}H-^{13}C 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

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 (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	T	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 i*sotopic 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 **11**
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.

Suggested Readings

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	T	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., $PbSO_4$, $BaSO_4$) conductometrically.
3. Determination standard electrode potential of Fe^{2+}/Fe^{3+} 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 H_3PO_4 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 $S_2O_8^{2-} + I^- \rightarrow SO_4^{2-} + I_2$.
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.

Suggested Readings

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	T	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 ^{1}H, ^{13}C 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 ^{1}HNMR 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	T	P	Cr
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 **4 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 **4 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 4
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 4
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	T	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, organo-lanthanides 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 **15**
Hours

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

NMR: Basic concepts of NMR with emphasis on ^{31}P, ^{19}F, ^{29}Si, ^{11}B, ^{10}B, ^{57}Se, ^{125}Te, ^{95}Mo, ^{109}Ag, ^{195}Pt, ^{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 Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (2) Sn^{2+} and Sn^{4+} 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 **10 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

Suggested Readings

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	T	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 **11 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, OsO_4, 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 **11 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 $NaBH_4$, Luche reduction, $NaBH_3CN$, L-selectride, K-selectride, $NaBH(OAc)_3$, $LiAlH_4$, DIBAL.

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

Unit 4 **12 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

·Suggested Readings

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

L	T	P	Cr
0	0	4	2

Course Title: Advanced Practical Chemistry
Paper Code: CHM.558
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 bio-macromolecules.

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)
   - dihydropyrimidinone (*via* Biginelli reaction)
   - propargylamine (*via* A^3-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.

Course Title: Advanced Logics in Chemistry	**L**	**T**	**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 **7 Hours**

Combined Structure problems: Exercises of structure elucidation of unknown compounds *via* combined spectral interpretation of IR, UV-vis, ^{1}H and ^{13}C NMR and mass spectra, along with two-dimensional NMR spectroscopy. IUPAC nomenclature of organic molecules including regio- and 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 **8 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.*

Unit 3 **7**
Hours

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

Suggested Readings

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.*

Course Title: Solid State Chemistry	L	T	P	Cr
Paper Code: CHM.560	3	0	0	3

Total Contact Hours: 45

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

- Physicochemical properties, defects in solid, diffraction techniques, electrical and magnetic properties of materials.
- The relationship between material structure and physical attributes associated with them.
- Advance applications of these materials.

Unit 1 **15Hours**

Solid State Structure: Primitive lattice vectors, reciprocal lattice, crystal systems and symmetry, Bravais lattices, lattice energy, crystal structure of diamond, NaCl, KCl, CsCl, TiO_2, etc.,

Defects: Intrinsic and extrinsic defects, point, line and plane defects, vacancies, Schottky defects, Frenkel defects, Thermodynamic and structural aspects.

Diffraction Methods: Basic concepts of X-ray, electron and neutron diffraction methods, structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase identification, X-ray structure analysis, XRD and its applications, polymorphism and cocrystallization.

Demonstration of characterization of these solid state materials like XRD.

Unit2 **10Hours**

Magnetic Materials (Ferrites) Introduction, structure and classification, Langevin diamagnetism, 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. Raman scattering in crystals, photoconduction, lasers, photovoltaic and photocatalytic effects.

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

Unit3 **10Hours**

Semiconductor and Superconductors: Band theory, band gap, metals and semiconductors, intrinsic and extrinsic semiconductors, p-n junctions and other applications (optical activity).

Debate on semiconductor materials and their optical and conduction character for device fabrication.

Unit4 **10 Hours**

Nanomaterials: Nanoparticles: zero dimensional nanostructure, homogeneous and heterogeneous nucleation, metallic nanoparticles-synthesis and applications; nanowires and nanorods: one dimensional nanostructures, spontaneous growth, VLS, electro spinning, lithography; thin film: two dimensional nanostructure- preparation techniques; Langmuir-Blodgett (LB) film growth techniques, photolithography properties and applications.

Brainstorming session on the properties of low dimension materials formation.

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

Suggested Readings

1. Ashcroft, N. W., and Mermin, N. D. (1976). *Introduction to Solid State Physics*. Saunders.
2. Callister Jr., W. D., and Rethwisch, D. G. (2012). *Fundamentals of Materials Science and Engineering: An Integrated Approach*. John Wiley and Sons.
3. Anderson, J. C., Leaver, K. D., Rawlings, R. D., and Leavers, P. S. (2004). *Materials Science for Engineers*. CRC Press.
4. Keer, H. V. (1993). *Principles of the Solid State*. New Age International.

Course Title: Polymer Chemistry	**L**	**T**	**P**	**Cr**
Paper Code: CHM.561	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 polymerization; their mechanism and role of initiator, chain transfer agent, solvent and inhibitor. Effect of structure of monomer on free-radical polymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems. Method for reaction rate determination using Rotating disk method and Pulsed Laser Photolysis – Size exclusion chromatography (PLP-SEC).

Learning use of various polymerization options by peer learning.

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.

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.

Understanding the polymer molecular mass estimation and distribution using problem solving approach.

UNIT III **11 Hours**

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.

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

Analysis of polymer processing parameters using brainstorming session.

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.

Game based and flipped learning of applications of polymers.

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

Suggested Readings

1. Carraher Jr, C. E. (2016). *Carraher's polymer chemistry*. 9th ed. CRC press.
2. Chanda, M. (2013) Introduction to polymer science and Chemistry: A Problem Solving Approach, 2nd ed., CRC Press.
3. Ebewele, R. O. (2000) Polymer Science and Technology, CRC Press.
4. Billmeyer, Jr., F.W. (2007). *Textbook of Polymer Science*. Wiley.
5. Odian, G. (2004). *Principles of Polymerization*. John Wiley and Sons.
6. Cowie, J. M. G., and Arrighi, V. (2007). *Polymers: Chemistry and Physics of Modern Materials*. CRC press.
7. Takemoto, K. Inaki Y. and Ottanbrite R.M. (1997). *Functional Monomers and Polymers,* CRC Press.
8. Gowariker, V. R., Viswanathan, N. V., and Sreedhar, J. (1986). *Polymer Science*. New Age International.
9. Alcock H.R., Lambe, F.W., and Mark, J. E., (2003). *Contemporary Polymer Chemistry*, Prentice Hall.
10. Peacock, A., and Calhoun, A. (2012). *Polymer Chemistry-Properties and Applications*. Hanser Publishers, Munich.
11. Bahadur, P., and Sastry, N. V., (2002). *Principles of Polymerization*, Narosa Publishing House, New Delhi.
12. Thomas, E. (2007) https://ocw.mit.edu/courses/materials- science-and-engineering/3-063-polymer-physics-spring-2007
13. 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: Inorganic Photochemistry	L	T	P	Cr
Paper Code: CHM.562	3	0	0	3

Total Contact Hours: 45

Learning Outcomes: The student will be able to

- Inorganic photochemistry and photophysical chemistry.
- The characterization of transient intermediates by ultrafast modern techniques.
- The theory of photoreaction.
- The photochemistry and photophysical chemistry of macromolecules.

Unit 1 **10 Hours**

Basics of Photochemistry: Electronic transitions, Jablonski diagram and photophysical processes, radiative transitions, absorption and emission, phosphorescence, intersystem crossing, mechanisms of singlet-triplet conversion (spin-orbit coupling), examples of ISC between states of different configurations, radiative rates, radiationless transitions, internal conversion, energy gap.

Brainstorming on identification of the various photophysical process where electronic transitions of inorganic molecules are relevant to achieve sustainable development.

Unit2 **10 Hours**

Photochemical Mechanism: Properties of excited states- structure, dipole moment, photochemical kinetics- calculation of rates of radiative process; bimolecular deactivation- quenching; excited states of metal complexes comparison with organic compounds, electronically excited states of metal complexes, charge transfer excitation.

Demonstration of the inorganic photochemical reactions and discussion on their potential use as a replacement for artificial photosynthesis.

Unit3 **10 Hours**

Ligand Field Photochemistry: Photosubstitution, photooxidation and photoreduction, ground state and excited state, energy content of the excited state, development of redox potentials of the excited states; redox reactions by excited metal complexes- energy transfer (FRET and SET), exciplex formation.

Discussion on recent variants of well-established photochemical process.

Unit4 **15 Hours**

Applications of Photochemistry: Measurement of fluorescence and phosphorescence and lifetimes, introduction to time-resolved techniques for absorption and emission measurements, detection and kinetics of reactive intermediates, photochromic reactions and memory devices, sensors, switches and molecular machines, TiO_2 photocatalysis, flash photolysis.

Application and challenges for the harvesting of energy via value added chemicals.

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

Suggested Readings

1. Lakowicz, J. R., (2006). *Principles of Fluorescence Spectroscopy*, Springer.
2. Rohatgi-Mukherjee, K. K., (1986). *Fundamentals of Photochemistry*. New Age International.
3. Kryukov, A. I., and Yakuchmii, S., (1990). *Fundamentals of Photochemistry of Coordination Compounds*.
4. Kavarnos, G. J. (1993). *Fundamentals of Photoinduced Electron Transfer*. Vch Pub.
5. Valeur, B., and Berberan-Santos, M. N. (2012). *Molecular Fluorescence: Principles and Applications*. John Wiley and Sons.
6. Turro, N. J., Ramamurthy, V., and Scaiano, J. C. (2012). *Modern Molecular Photochemistry of Organic Molecules*. Wiley Publishers.
7. Ninomiya, I., and Naito, T. (2012). *Photochemical Synthesis*. Academic Press.

Course Title: Organotransition Metal Chemistry	**L**	**T**	**P**	**Cr**
Paper Code: CHM.576	3	0	0	3

Total Contact Hours: 45

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

- The chemistry of transition metal complexes and compounds of transition metal-carbon multiple bonds
- Chemistry on alkyls and aryls of transition metals and fluxional organometallic compounds
- Workout on homogeneous catalysis with appropriate planning.

Unit 1

10 Hours
Compounds of Transition Metal-Carbon Multiple Bonds: Metal Carbenes (Alkylidenes) and carbynes (alkylidynes) complex-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reaction on the ligands, role in organic synthesis.

Brainstorming on logistics behind formation and stability of various transition metals compounds.

Unit 2 15 Hours
Aliphatic Transition Metal Complexes: Transition metal complexes with alkyl and unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, and trienyl complexes, preparations, properties, nature of bonding and structural features important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Group discussion on stability and reactivity of Main group element vs Transition metal complexes with alkyl and unsaturated organic molecules.

Unit 3
10 Hours
Aryls Transition Metal Complexes: Types, routes of synthesis, stability and decomposition pathways, applications in organic synthesis.

Discussion on recent variants of well-established transition metal catalyzed reactions.

Unit 4
10 Hours
Homogeneous Catalysis: homogeneous catalytic hydrogenation, Zeigler-Natta catalyst and stereospecific polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction) oxo-palladation reactions, activation of C-H bond.

Peer group discussion on Transition metal based industrial processes.

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

Suggested Readings

1. Collman, J. P., Norton, J. R., Hegsdus, L. S. and Finke, R. G., (1987) *Principles and Application of Organotransition Metal Chemistry*. University Science Books.
2. Crabtree, R. G. (2011). *The Organometallic Chemistry of the Transition Metals*. John Wiley.
3. Mehrotra, R. C., and Singh, A., (2005). *Organometallic Chemistry*. New Age International.
4. Cotton, F. A., and Wilkinson, G., (1999). *Advanced Inorganic Chemistry*. John Wiley.
5. Pearson, A.J., (1985). *Metallo-Organic Chemistry*. Wiley.

6. Wu, X.-F., Neumann, H., and Beller, M., Synthesis of Heterocycles via Palladium-Catalyzed Carbonylations. Chemical Reviews 2013, 113, 1, 1-35.

7. Patil, N. T., and Yamamoto, Y., Coinage Metal-Assisted Synthesis of Heterocycles. Chemical Reviews 2008, 108, 8, 3395-3442.

Course Title: Current Trends in Organic Synthesis	**L**	**T**	**P**	**Cr**
Paper Code: CHM.579	3	0	0	3

Total Contact Hours: 45

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

- Know the potential of free radical chemistry for various coupling reactions including metal-free C-H bond activation/ functionalization.
- Apply the concept of enolate chemistry for controlling the selectivity of various organic transformations.
- Design various processes for the synthesis of commercially important molecules taking into consideration the protection and deprotection strategies.

Unit 1
11 Hours
Free radical reactions: Types of free radical reactions, free radical substitution mechanism at an aromatic substrate, free radical rearrangement, neighbouring group assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, Reactivity in the attacking radicals, the effect of solvents on reactivity, auto-oxidation. Coupling of alkynes and arylation of aromatic compounds by diazonium salts. Recent trends in oxidative functionalization of C-H bond *via* free radical chemistry.

Brainstorming on identification of free radical quenching reagents and role of free radicals in daily life.

Unit 2 **11 Hours**

Enolate Chemistry: Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, effect of solvent, counter-cation and electrophiles; symbiotic effect; thermodynamically and kinetically controlled enolate formations; various transition state models to explain stereoselective enolate formation; enamines and metallo-enamines; regioselectivity in generation, application in controlling the selectivity of alkylation.

Group discussion on stereoselective generation of enolates and alkylation in organic synthesis.

Unit 3 **11 Hours**

Protection and deprotection of various functional groups: Protection of alcohols by ether, silyl ethers and ester formations and their deprotection, protection of carbonyls by acetal and ketal formation and their deprotection, protection of 1, 2 diols- by acetal, ketal and carbonate formation and their deprotection, protection of amines by acetylation, benzylation, benzyloxy carbonyl, *t*-butoxycarbonyl (Boc), fmoc, triphenyl methyl groups and their deprotection, protection of carboxylic acids by ester formation and their deprotection: Recent advances in protection-deprotection free organic synthesis.

Demonstration on the role of protecting groups in synthesis of commercial drugs.

Unit 4

12 Hours

New synthetic reactions: 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, Shapiro reaction, Stork-enamine reaction, Aza-Cope, Aza-Wittig reaction, Ugi reaction, Robinson–Gabriel synthesis, Vilsmeier–Haack reaction.

Peer group discussion on well-established and newly developed synthetic approaches including recent variants and advantages associated with them.

Debate on various C-C and C-N bond forming and multicomponent reactions.

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

Suggested Readings

1. Finar, I. L., (2012). *Organic Chemistry Vol. 1*. Pearson Education, UK.
2. Finar, I. L., (2012). *Organic Chemistry Vol. 2: Stereochemistry and the Chemistry of Natural Products*. Pearson Education, UK.

3. Fleming I., (2011). *Molecular Orbitals and Organic Chemical Reactions*. John Wiley and Sons.
4. Li, J. J., (2014). *Name Reactions: A Collection of Detailed Reaction Mechanism*. Springer-Verlag.
5. Kalsi, P. S. (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub.
6. McMurry, J. (1996). *Organic Chemistry*, Brooks Cole.
7. Mukherjee, S. M., and Singh, S. P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd.
8. Smith, M. B., (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*. John Wiley and Sons.
9. Solomon, T. W. G., Fryhle, C. B. and Snyder, S. A., (2013). *Organic Chemistry*. John Wiley and Sons, Inc.
10. Sykes, P. A. (1997). *Guide Book to Mechanism in Organic Chemistry*. Prentice Hall.
11. Carruthers, W. (2004). *Some Modern Methods of Organic Synthesis*. Cambridge Uni. Press, UK.
12. Meyer, C. C., Ortiz, E., and Krische, M. J. Catalytic Reductive Aldol and Mannich Reactions of Enone, Acrylate, and Vinyl Heteroaromatic Pronucleophiles. Chemical Reviews 2020, 120, 8, 3721-3748
13. Schettini, R., & Della Sala, G. (2021). New Trends in Asymmetric Catalysis. *Catalysts*, 2021, 11, 306.
14. Dénès, F., Pérez-Luna, A., and Chemla, F., Addition of Metal Enolate Derivatives to Unactivated Carbon-Carbon Multiple Bonds. Chemical Reviews, 2010, 110, 2366-2447.
15. Mas-Torrent, M., Crivillers, N., Rovira, C., and Veciana, J., Attaching Persistent Organic Free Radicals to Surfaces: How and Why? Chemical Reviews 2012, 112, 2506-2527.

Course Title: Green Chemistry
Paper Code: CHM.520
Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Learning outcome: Students will be able to

- Differentiate various aspects of green chemistry for sustainable development
- Utilize ionic liquids, water and solid supported reaction conditions to reduce or eliminate use of volatile organic solvents
- Utilize energy efficient MW and ultrasonicaton in organic synthesis
- Apply the judicious use of green reagents for the environmental friendly synthesis of value added chemicals

Unit 1 **12 Hours**

Introduction to green chemistry: History, need and goals. Green chemistry and sustainability, dimensions of sustainability, limitations/obstacles in pursuit of the goals of green chemistry. Opportunities for the next generation of materials designers to create a safer future. Basic principles 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. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents, designing biodegradable products, Prevention of chemical accidents, Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

Group project on various green process successfully employed in chemical industries
Green chemistry is not costly: Classroom debate
Chemistry and sustainable lifestyle: Peer Discussion

Unit 2 **11 Hours**

Green Solvents: Role of solvents in chemical synthesis, Environmental and health concerns of organic solvents, need for alternative/cleaner solvents, Criteria for selection and design of green solvents Water: the natural solvent on earth, organic reactions: hydrophobic effects enhancing the reaction selectivities, low solubility of O2 in water, water soluble catalysts, challenges in using water as solvent,
Ionic liquids: physicochemical properties, Synthesis of Ionic Liquids, Directed Inorganic and Organometallic Synthesis, formation of oxides, electrochemical synthesis in ionic liquids,

Glycerol: solvent properties, volatility, polarity, availability, glycerol as a solvent combining the advantages of water and ionic liquids, enhancement of reaction selectivity, glycerol as a solvent for catalyst design and recycling, separation processes and material synthesis in glycerol, examples of synthesis of transition metal and metal oxide crystals

Supercritical fluids: supercritical CO_2 and its properties, advantages of using CO_2 as solvent, Synthesis of metal nanoparticles, CO_2 as solvent for coatings and lithography, biomaterial processing, other supercritical fluids.

Industrial applications of green solvents: peer discussion in the classroom
Project work on most polluting chemical industries
Debate on the single use plastic

Unit 3 **11 Hours**

Microwave induced and ultrasound assisted green synthesis: Introduction to synthetic organic transformation under microwave (i) Microwave assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave solvent free reactions Ultrasound assisted reactions: Introduction, substitution reactions, addition, oxidation, reduction reactions. Biocatalysts in organic synthesis: Introduction, Biochemical oxidation and reductions.

Modern tools as source of energy for chemical reactions

Unit 4 **11 Hours**

Approaches to green synthesis: Use of green reagents: polymer supported reagents: peptide coupling reagents. Green catalysts, Phase-transfer catalysts in green synthesis. Advantages of PTC, Application of PTCs in C-alkylation, N-alkylation, S-alkylation. Darzens reaction, Williamsons synthesis, Wittig reaction, Click Chemistry. Use of Crown ethers in esterification, saponification. Micellar catalysis, Biocatalysis.

Role of Green reagents and their applications for the synthesis of diverse scaffolds through peer learning
Implication and challenges of Biocatalysis in industrial setting through group presentation.

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

Suggested Readings:

1. Anastas, P., Crabtree, R. H. (2013, 9th edition), *Handbook of Green Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA

2. Ahluwalia, V. K.; Kidwai M. (2004). *New Trends in Green Chemistry*, Springer

3. Anastas, P.T.; Warner J. C. (2005, reprint edition). *Green chemistry, Theory and Practical*. Oxford University Press, UK.
4. Grieco, P.A. (1998). *Organic Synthesis in Water*. Publisher: Springer.
5. Wasserscheid, P., and Welton, T., (2008), *Ionic Liquids in Synthesis*, WILEY-VCH Verlag GmbH & Co. KGaA.
6. Sheldon, R.A., Arends, I. and Hanefeld U. (2007), *Green Chemistry and Catalysis*, WILEY-VCH Verlag GmbH & Co. KGaA.
7. William M. N.; (2003) *Green Solvents for Chemistry*: *Perspectives and Practice*, Oxford University Press.
8. Zhigang Lei, Biaohua Chen, Yoon-Mo Koo, and Douglas R. MacFarlane; Introduction: Ionic Liquids, *Chem. Rev.* 2017, 117, 10, 6633–6635
9. Peter Priecel and Jose Antonio Lopez-Sanchez, Advantages and Limitations of Microwave Reactors: From Chemical Synthesis to the Catalytic Valorization of Biobased Chemicals; Peter Priecel *ACS Sustainable Chem. Eng.* 2019, 7, 1, 3–21.

Course Title: Advanced Organic Synthesis	**L**	**T**	**P**	**Cr**
Paper Code: CHM.574	3	0	0	3

Total Contact Hours: 45

Learning Outcomes: The students will be able to

- Identify various asymmetric tools for the synthesis of chiral compounds.
- Design the synthesis of alkenes and functionalized molecules utilizing phosphorus, nitrogen and sulphur ylides.
- Explore various reagents for functional group conversions and synthesis of organic frameworks.

Unit 1 **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, chemo-regio- and stereoselective transformations, organocatalysis and biocatalysis.

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

Unit 2
11 Hours
Reaction of ylides: Phosphorus ylide; structure and reactivity, stabilized ylides, effects of ligands on reactivity, Witting, Wittig-Horner and Wadsworth Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification. Sulphur ylides; stabilized and non-stabilized ylides: thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions. Nitrogen Ylides; Stevens rearrangement, Sommelet-Hauser rearrangement. Peterson's olefination.

Peer group discussion on various methods to construct double bonds (including exocyclic double bonds) and respective advantages.

Unit 3 **11 Hours**
Organometallic compounds: Organoboranes: Preparation of organoboranes viz hydroboration with BH_3-THF, dicyclohexylborane, disiamylborane, thexylborane, 9-BBN catalyzed hydroboration, functional group transformations of organoboranes: oxidation, protonolysis and rearrangements, formation of carbon-carbon-bonds *viz* organoboranes carbonylation. Chiral Organobornaes: diisopinocampheyl borane, alpine borane.
Applications of organolithium, organozinc, organosilicon, organopalladium and organostannous compounds in C-C coupling reactions.

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

Unit 4 **12 Hours**
Reagents in organic synthesis: Gilman's reagent, Lithium diisopropylamide (LDA), 1,3-Dithiane (Umpolung reagent), Trimethylsilyl iodide, Baker's yeast, Woodward and Prevost reagents, Crown ether, Merrifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawsson reagent, IBX, Fetizon reagent, Dioxiranes, Tebbe reagent, Corey-Nicolaou reagent and macrolactonization, Mosher's reagent.

Comparison on the reactivity and selectivity of various reagents through collaborative learning.

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

Suggested Readings

1. Kalsi, P. S. (2020). *Organic Reactions and Their Mechanism*. New Age International Publisher, India; 5th edition.
2. Li, J. J., (2021). *Name Reactions: A Collection of Detailed Reaction Mechanism*. Springer; 6th edition.
3. Mundy, B. P., Ellerd, M. G., and Favaloro Jr, F. G., (2005). *Name Reactions and Reagents in Organic Synthesis*. John Wiley and Sons; 2nd edition.
4. Claydon, J., Gleeves, and N., Warren, S., (2014). *Organic Chemistry*. Oxford University Press, UK; 2nd edition.
5. Yadav, L. D. S., Singh, J., and Singh, J. (2017). Organic Synthesis, Pragati Prakashan, India.
6. Norman, R. O. C., and Coxon, J. M. (2017). Principle of Organic Synthesis, CRC Press; 3rd edition.
7. Finar, I. L., (2012). *Organic Chemistry*. Pearson Education, UK.
8. Smith, M. B., (2020). *March's Advanced Organic Chemistry: Reactions, Mechanisms, And Structure*. John Wiley and Sons; 8th edition.
9. Corey, E.J. and Cheng, X.-M. (2011). *The Logic of Chemical Synthesis*. John Wiley and Sons.
10. Fuhrhop, J. H., Penzlin, G., and Li, G., (2003). *Organic Synthesis: Concepts and Methods*. John Wiley and Sons.
11. Davies, S. G., (2013). *Organotransition Metal Chemistry: Applications to Organic Synthesis: Applications to Organic Synthesis* (Vol. 2). Elsevier.
12. Aitken, A., and Kilényi, S. N., (Eds.). (2012). *Asymmetric Synthesis*. Springer.
13. 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*.
14. Schettini, R., & Della Sala, G. (2021). New Trends in Asymmetric Catalysis. *Catalysts*, 2021, 11, 306.
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. Farina, V., Reeves, J. T., Senanayake, C. H. and Song, J. J., Asymmetric Synthesis of Active Pharmaceutical Ingredients, Chemical Reviews, 2006, 106, 7, 2734-2793.

Course Title: Bioinorganic and Biophysical Chemistry
Paper Code: CHM.553
Total Contact Hours: 45

L	T	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 **11 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 **12 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 **11 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 **11 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. andSchimmel, 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.

L	T	P	Cr
3	0	0	3

Course Title: Chemistry of Natural Products
Paper Code: CHM.575
Total Contact Hours: 45

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

- Recognize various types of natural products and their importance.
- Identify various types of natural products including their properties, occurrence, structure and biosynthesis.
- Apply the knowledge of natural product synthesis in drug development

Unit 1 **11Hours**

Terpenoids and Carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Geraniol, Menthol and β-Carotene and biological activities.

Importance of isoprene rule in the biosynthesis of terpenes through group presentation

Advances of terpene based drugs through peer learning

Unit 2
11Hours
Alkaloids: Nomenclature and physiological action, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, structure, stereochemistry, synthesis of the following: Ephedrine, Nicotine, Morphine Reserpine and general theory of biogenesis.

Class room debate on theory of biogenesis of alkaloids
Group project on structure-activity relationship based on alkaloid structures

Unit 3
11Hours

Steroids: Occurrence, nomenclature, basic skeleton and stereochemistry, structure determination and synthesis of cholesterol, partial synthesis of testosterone and progesterone, chemical tests for steroids and biological activities.

Coumarins and lignans: Classification, isolation, stereochemistry, biological activity, biosynthesis and synthesis of lignans.

Group presentation on biological importance of steroids and lignans

Peer learning of pharmacophore model of natural products

Unit 4
12Hours

Plant pigments: Occurrence, nomenclature and general methods of structure determination. isolation, synthesis and biological activities of anthocyanins, chlorophyll.

Carbohydrates: Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of glucose, conformation and anomeric effects in hexoses. Mono, di, oligo- and polysaccharides, separation and isolation, purification, structure determination, biological activity.

Group presentation on biological importance of plant pigments

Class room debate on structures and conformation of carbohydrates

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

Suggested Readings

1. Bhat, S.V., Nagasampagi, B.A., andMeenakshi, S. (2009). *Natural Product Chemistry and Applications*.Narosa Publishing House, New Delhi.
2. Bhat, S.V., Nagasampagi, B.A., and Sivakumar, M. (2005). *Chemistry of Natural Products*. Narosa Publishing House, New Delhi.
3. Cseke, L.J., (2009). *Natural Products from Plants*.CRC Press.
4. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Wiley and Sons,UK.
5. Finar, I.L., (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Dorling Kindersley Pvt. Ltd., India.
6. Peterson, F. and Amstutz, R., (2008). *Natural Compounds as Drugs*. Birkhauser-Verlay.
7. Daley. S. K., Cordell, G. A., Biologically Significant and Recently Isolated Alkaloids from Endophytic Fungi, *J. Nat. Prod.* 2021, 84, 3, 871–897.
8. 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.

9. Ramabulana, T., Scheepers, L.M., Moodley, T., Maharaj, V. J., Stander, A., Gama, N., Ferreira, D., Sonopo,M.S., Selepe, M.A. Bioactive Lignans from *Hypoestes aristata, J. Nat. Prod. 2020, 83, 8, 2483–2489.*

L	T	P	Cr
3	0	0	3

Course Title: Supramolecular Chemistry
Paper Code: CHM.580
Total Contact Hours: 45

Learning Outcome: The students will acquire knowledge of

- Various supramolecular aspects of interaction between two chemical systems.
- Devising supramolecular systems based on complementarity and preorganizational requirements of host.
- Analyze design of hosts for functions based on supramolecular assembly using complementarity and preorganization.
- Interpret the basic designs of supramolecular machines

Unit 1 **11 Hours**

Introduction: Definition and development of supramolecular chemistry, nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-π, anion- π, π -π and van der Waals interactions. Supramolecular chemistry in life, ionophores, porphyrin and other tetrapyrrollic macrocycles, coenzymes, neurotransmitters, DNA and biochemical self-assembly. Pre-organization and complementarity, receptors, nature of supramolecular interactions.

Host-guest chemistry: synthesis and structure of crown ethers, lariat ether and podands, cryptands, spherands, calixarenes, cylcodextrins, cyclophanes, carcerands and hemicarcerands. Concepts of selectivity, macrocyclic, macrobicyclic synthesis and template effects,

Unit 2 **11 Hours**

Cation Binding: Binding Constant and its determination, concept of coordination chemistry, cation complexation using various preorganized host, soft ligands including N, S and P based macrocycles, Schiff's base, proton and ammonium ion complexation, carbon donor and π- acid ligands, siderophores.

Anion Receptor: Anion recognition and its biological relevance, concepts on anion host design, from cation to anion hosts- a simple change in pH, guanidinium- based receptors, neutral receptors, organometallic receptors, coordination interactions. Chromogenic and fluorogenic receptors, dosimeters, ion pair recognition and zwitterion recognition.

Innovating receptor designs for challenging and emerging sensing application through team work and brainstorming.

Unit 3 **11 Hours**

Molecular Self-assembly: Supramolecular polymers: definition, kinetic and thermodynamic consideration of self-assembly. self-assembly molecules: design, synthesis and properties of the molecules, self-assembly by H-bonding, proteins and foldamers, DNA, catenanes, rotaxanes, molecular knot: topology and examples including trefoil and borromean rings, surfactants self-assembly, liquid crystals.

Dendrimers structure and nomenclature, synthesis and characterization, supramolecular chemistry of dendrimers and its assembly, dendritic nanodevices

Supramolecular polymers including amphiphilic block polymers and molecular imprinter polymers, biological self-assembly in amyloids, actins and fibrin, COF and supramolecular gels.

Using supramolecular synthons for building self-assembled motif for purpose by peer learning.

Unit 4 **12 Hours**

Supramolecular and Molecular Devices: Supramolecular photochemistry and catalysis, molecular electronic devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches and molecular logic gates, organics for photonics and electronics.

Molecular Machines: Molecular machine terminology and bio-inspiration, ratchet mechanism including pulsating and tilt mechanism, covalent and supramolecular motors and their controlling mechanisms, machines based on catenanes and rotaxanes. Applications as molecular walkers, switchable catalysts, surface analysis at molecular dimensions.

Hands on exercise in groups to develop a theoretical design of a machine tool using organic synthons in supramolecular chemistry.

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

Suggested Readings

1. Steed, J. W., and Atwood, J. L. (2013). *Supramolecular chemistry*. John Wiley and Sons.
2. Lehn, J. M., (1995). *Supramolecular Chemistry-Concepts and Perspectives*. Wiley –VCH.

3. Beer, P.D., Gale, P. A., and Smith, D. K., (1999). *Supramolecular Chemistry*. Oxford University Press.
4. Martin, N. and Nierengarten, J.-F. (2012). *Supramolecular Chemistry of Fullerenes and Carbon Nanotubes*. Wiley-VCH.
5. Vicens, J. and Harrowfield, J. (2007). *Calixarenes in the Nanoworld*. Springer.
6. Schalley, C. A. (2012). *Analytical Methods in Supramolecular Chemistry*. Vol. 1 and 2, Wiley-VCH.
7. Erbas-Cakmak, S., Leigh, D. A., McTernan, C. T., and Nussbaumer, A. L. (2015). Artificial molecular machines. *Chemical Rev*iew,*115*(18), 10081-10206.
8. Kubik, S. (2020) Supramolecular Chemistry: From Concepts to Applications, De Gruyter.
9. Dequan, A. L., (2013) Molecular Self-Assembly: Advances and Applications, CRC Press.
10. Ferringa, B.-L., Browne, W.R. (2011) Molecular Switches, Wiley Publishing.
11. Baruah, J. B. (2017) Concepts for Molecular Machines, World Scientific Publishers Co.
12. Hoffmann, P. M. (2012) Life's Ratchet: How Molecular Machines Extract Order from Chaos, Basic Sciences Publishing.

Course Title: Medicinal Chemistry-I

Paper Code: CMC.510

Course Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes

After completing this course, the learner will be able to:

- Interpret basics concepts of drugs, their effects and screening.
- Describe drugs interaction with various types of enzymes and receptors
- Conceptualize the process of drug discovery and its progress

Unit 1 **10 hours**

History of drug discovery Introduction, Drug discoveries, Recent trends in drug discovery, Enzymes as drug targets, Membrane transporters as drug targets, Voltage-gated ion channels as drug targets

· *Learner will be engaged in group discussion to explain history of drug discovery*

Unit 2 **11 hours**

Drug discovery:

Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets

Biological drug targets

Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonist vs antagonists, artificial enzymes.

Measurement and expression of drug effects

Introduction, *In-vitro* experiments, *Ex-vivo* experiments, *In-vivo* experiments.

Learner will be explained about drug interaction and target through molecular modeling studies

Unit 3 **12 hours**

Prodrug Design and Analog design

Prodrug design

Basic concept, Carrier linked prodrugs/ Bioprecursors, Prodrugs of functional group, Prodrugs to improve patient acceptability, Drug solubility, Drug absorption and distribution, site specific drug delivery and sustained drug action. Rationale of prodrug design and practical consideration of prodrug design.

Combating drug resistance

Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance.

Analog Design

Introduction, Classical & Non classical, Bioisosteric replacement strategies, rigid analogs, alteration of chain branching, changes in ring size, ring position isomers, design of stereo isomers and geometric isomers, fragments of a lead molecule, variation in inter atomic distance.

Learner will be engaged in Web based training to familiarize with prodrug and analog design

Unit 4
12 hours

a) Medicinal chemistry aspects of the following class of drugs Systematic study, SAR, Mechanism of action and synthesis of new generation molecules of following class of drugs:

b). Anti-hypertensive drugs, Psychoactive drugs, Anticonvulsant drugs, H1 & H2 receptor antagonist, COX1 & COX2 inhibitors, Adrenergic & Cholinergic agents, Antineoplastic and Antiviral agents.

c). Stereochemistry and Drug action: Realization that stereo selectivity is a pre-requisite for evolution. Role of chirality in selective and specific therapeutic agents. Case studies, enantioselectivity in drug adsorption, metabolism, distribution and elimination.

Learner will be engaged in Group discussion to explain SAR, Mechanism of action and synthesis of drugs

Suggested Readings:

1. Foye, W. C. (2019). *Principles of Medicinal Chemistry*, Publisher: Wolters Kluwer.
2. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royal Society of Chemistry.
3. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press.
4. Patrick, G.L. (2017). *An Introduction to Medicinal Chemistry*, Publisher: Oxford university Press, UK.
5. Singh, H., Kapoor, V.K. *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
6. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis.
7. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
8. Wolff, M E, Ed., (Latest Edition). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley and Sons, New York.
9. Ferrant, E., (2011). *New Synthetic Technologies In Medicinal Chemistry*. Royal Chemical Society.
10. Medicinal Chemistry by Burger, Vol I –VI.

11. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, 12th Edition, Lppincott Williams & Wilkins, Woltess Kluwer (India) Pvt.Ltd, New Delhi.
12. Comprehensive Medicinal Chemistry – Corwin and Hansch.
13. Computational and structural approaches to drug design edited by Robert M Stroud and Janet. F Moore

The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Team teaching

Transaction Mode

- Molecular Models
- PPT
- YouTube
- Software for *In silico* study
- Google meet

Course Title: Fundamentals of Computer Aided Drug Design **Paper Code: CMC.52**	**L**	**T**	**P**	**Credits**
	3	0	0	3

Course Hours: 45h

Learning outcome:

After completing this course, the learner will be able to:

- Describe the role of CADD in drug discovery
- Design and develop new drug like molecules
- Work with molecular modelling software's to design new drug molecules

Unit 1 **12 hours**

Introduction to Computer Aided Drug Design (CADD): History, different techniques and applications. Quantitative Structure Activity Relationships: Basics. History and development of QSAR: Physiochemical parameters and methods to calculate physiochemical parameters: Hammett equation and electronic parameters (sigma), lipophilicity effects and parameters (log P, pi-substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physiochemical parameters. Hansch analysis, Free Wilson analysis and relationship between them, Advantages and disadvantages: Deriving 2D-QSAR equations. 3D- QSAR approaches and contour map analysis. Statistical methods used in QSAR analysis and importance of statistical parameters.

- *Learner will be engaged in group discussion to explain 2D-QSAR, 3D-QSAR and importance of statistical parameters*

Unit 2 **11 hours**

Molecular Modeling and Docking:

a) Molecular and Quantum Mechanics in drug design.

b) Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation.

c) Molecular docking and drug receptor interactions: rigid docking, flexible docking and extra-precision docking. Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AchE & BchE)

Learner will be engaged in molecular modeling of compounds

Unit 3 **10 hours**

Molecular Properties and Drug Design:

a) Prediction and analysis of ADMET properties of new molecules and its importance in drug design.

b) De novo drug design: Receptor/enzyme-interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design.

c) Homology modelling and generation of 3D-structure of protein.

- *Learner will study Molecular model to explain interactions between ligand and drug target*

Unit 4 **12 hours**

Pharmacophore Mapping and Virtual Screening: Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophores modelling; Conformational search used in pharmacophore mapping. In-silico Drug Design and Virtual Screening Techniques. Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols.

- *Learner will be engaged in Pharmacophore band structure based In-silico virtual screening protocols*

Suggested Readings

1. Ellis, G.P., West, G. B. (1983). *Progress in Medicinal Chemistry Series*. Elsevier Science.
2. Foye, W.O., Lemke, T. L., Williams, D. A. (2019). *Principles of Medicinal Chemistry*, Indian Ed. Waverly, Pvt. Ltd. New Delhi.
3. Ganellin, C.R.; Roberts S. M., (1993). *Medicinal Chemistry: The Role of Organic Chemistry in Drug Research*. Publisher: Academics Press Inc.
4. Kadam, Mahadik, Bothara (2010). *Principle of Medicinal Chemistry (Volume I & II)*, Nirali publication
5. Kulkarni, V. M., Bothra, K.G., (2008). *Drug Design*, Nirali Publication.
6. Lawton, G., Witty, D.R. (2011). *Progress in Medicinal Chemistry Series. Volume 50*.
7. Lednicer D., Laster A. M. (1998). *The Organic Chemistry of Drug Synthesis (3 Volumes)* John Wiley & Sons.
8. Lednicer, D. (2008). *Strategies for Organic Drug Synthesis and Design. (7 volume)* Publisher: John Wiley & Sons.
9. Lemke, T.L., Williams, D.A. (2012). *Foye's Principles of Medicinal Chemistry*.
10. Silverman R.B., (2014). *Organic Chemistry of Drug Design and Drug Action*, Publisher: Elsevier.
11. Wilson, C.O.; Block, J.H.; Gisvold, O.; Beale,J. M. Wilson and Gisvold's (2003) *Textbook of Organic Medicinal and Pharmaceutical Chemistry*. Lippincott Williams & Wilkins.
12. Gore, M., & Jagtap, U. (2018). *Computational Drug Discovery and Design*. Springer Publishers.

The following are some of the modes of classroom transaction

- Lecture
- Group discussion
- Demonstration
- Team teaching

- Tutorial
- Self-learning

Transaction Mode

- PPT
- YouTube
- Molecular modeling software
- Google drive
- Google meet

L	T	P	Cr
3	0	0	3

Course Code: BCH.508

Course Title: Biomolecules and Bioenergetics

Total Hours: 45

Learning outcomes: Students will be able to

- Demonstrate the concepts of biomolecules and bioenergetics, various components of cells which are essential for energy generation and their biosynthesis.
- Apply and effectively communicate scientific reasoning and data analysis in both written and oral forums related to biomolecules and energetics of biochemical processes.
- Describe and correlate biomolecules and bioenergetics

Unit I **10**
Hours Carbohydrate: Classification, structure, stereochemistry, chemical properties epimerization, anomerization and mutarotation and reaction of carbohydrates, functions of polysaccharides starch, glycogen, cellulose and chitin, complex carbohydrates; amino sugars, proteoglycans and glycoproteins.
Lipids: Classification, structure, properties and functions of fats and fatty acids, essential fatty acids, phospholipids, sphingolipids, cerebrosides, steroids, bile acids, prostaglandins, lipoproteins, proteolipids,

phosphatidopeptides, lipopolysaccharides. Peer discussion on the existence of these biomolecules in different organisms.

Unit II **12 Hours**

Buffers and Proteins: Classification, structure and properties of amino acids. The concept of pH, dissociation and ionization of acids and bases, pKa, buffers and buffering mechanism, Henderson Hasselbalch equation, ionization of amino acids and proteins, measurement of pH. Classification and properties of proteins, sequencing of proteins Primary (peptide conformation, N- and C-terminal, peptide cleavage), Secondary (α-helix, sheet, random coil, Ramachandran plot), Tertiary and Quaternary structures of proteins. Thermodynamics of Protein folding, coagulation and denaturation of proteins. Presentations on buffers and proteins properties and its constituents.

Unit III **10 Hours**

Nucleic acids: Structure of purines, pyrimidines, nucleosides and nucleotides. Structure, types and biological role of RNA and DNA. Primary, secondary, and tertiary structure of nucleic acids, DNA forms and conformations, UV absorption and Denaturation of DNA, C-value paradox, Cot curve analysis. In depth discussion on the role of DNA modification and its effects.

Unit IV **10 Hours**

Bioenergetics: Laws of Thermodynamics, Concept of free energy, standard free energy, determination of ΔG for a reaction. Relationship between equilibrium constant and standard free energy change, standard free energy change in coupled reactions. Biological oxidation-reduction reactions, redox potentials, relation between standard reduction potentials & free energy change. High energy phosphate compounds – introduction, phosphate group transfer, free energy of hydrolysis of ATP and sugar phosphates along with reasons for high ΔG. Group discussion on analysis of thermodynamic parameters.

Suggested Readings:

1. Outlines of Biochemistry. Eric E. Conn and Paul K. Stumpf (2006). 5th edition John Wiley and Sons, India edition.
2. Davidson, VL and Sittman, DB (1999) *Biochemistry* NMS, 4th ed. Lippincott. Willams and Wilkins.
3. Voet, D and Voet JG (2010) *Biochemistry*, 4th ed. Wiley
4. Rodwell V, Bender D, Botham KM, Kennelly PJ and Weil PA (2018) *Harper's Illustrated Biochemistry.* 31st ed. McGraw Hill.
5. Berg JM, Stryer L, Tymoczko JL, Gatto GJ (2018) *Biochemistry*, WH Freeman, 9th ed.

6. Lodish, H, Birk, A, et al. (2016) *Molecular Cell Biology*. 8th ed. WH Freeman.
7. Nelson DL and Cox MM (2017) *Lehninger's Principles of Biochemistry*, 7th ed. WH Freeman.

Web resources:

- https://nptel.ac.in/courses/104/103/104103121/
- https://www.youtube.com/watch?v=iuW3nk5EADg
- https://www.youtube.com/watch?v=ZqoX2W1N6l0
- https://www.youtube.com/watch?v=DhwAp6yQHQI
- https://www.youtube.com/watch?v=jLyi2K-29xU
- https://www.youtube.com/watch?v=C0ky85Kk2Zc
- https://www.youtube.com/watch?v=Fp1wKo72b2A
- https://www.youtube.com/watch?v=zOO5qdpl24I

Modes of transaction

-Lecture cum Demonstration
-Problem solving approach
-Self-Learning
-Inquiry training
-Co-operative learning

Tools used

PPT, You tube Video, Google meet, NPTE

L	T	P	Cr
0	0	8	4

Course Title: Research Proposal
Paper Code: CHM.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	T	P	Cr
0	0	40	20

Course Title: Dissertation
Paper Code: CHM.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	T	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 **7 Hours**

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 **7 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 **8 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 7 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 (TiO_2, CeO_2, 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 8 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, H_2 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**	**T**	**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 **7 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 **7 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 **9 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	T	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 **7 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.

Suggested Readings

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/wqmchap9.pdf
4. https://www.unece.org/fileadmin/DAM/env/water/publications/documents/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 Publlishing.
12. Hasnain, M.S., Beg, S., (2019) Pharmaceutical Quality by Design: Principles and Applications, Elsevier Science.

L	T	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 **7 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 **7 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

Suggested Readings

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	L	T	P	Cr
Paper Code: CHM.528	2	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 **8 Hours**

Structure and function of hemoglobin, myoglobin and transferrin; Iron metabolic disorders (anemia, Sickle cell anemia, thalassemia, hemochromatosis), Diabetes; Types of diabetes and 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

Suggested Readings

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			**L**	**T**	**P**	**Cr**
Paper Code: CHM.531			2	0	0	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 Mg^{2+} 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

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*. 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.

L	T	P	Cr
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 **8 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.
^{13}C NMR Spectroscopy.

Interpretation of various peaks for structural identification through demonstration of various ^{1}H and ^{13}C 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

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 (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.