

Central University of Punjab



Course Structure and Syllabus

M.Sc. Chemistry

Batch 2025-27

Department of Chemistry

School of Basic Sciences

Graduate Attributes

Graduate attributes are the understanding, skills, and qualities that Department of Chemistry along with CUPB community agrees with where the M. Sc. Chemistry students should develop these characteristics during the time spent in the institution.

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 behavior and have entrepreneurial potential and will be able to take leadership roles in their occupations, careers and community with ethical behavior. 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.	Course Code	Course Title	Course Type	L	T**	P	Cr
1	MCHM.401	Transition Metal Complexes and Reaction Mechanism	DSC	3	0	0	3
2	MCHM.402	Reaction Mechanism and Stereochemistry	DSC	3	0	0	3
3	MCHM.403	Quantum Chemistry	DSC	3	0	0	3
4	MCHM.404	Spectroscopic Techniques	DSC	3	0	0	3
5	MCHM.405	Thermodynamics, Kinetics and Electrochemistry	DSC	3	0	0	3
6	MCHM.406	Inorganic Chemistry (Practical)	SEC	0	0	4	2
7	MCHM.407	Organic Chemistry (Practical)	SEC	0	0	4	2
8	MCHM.408	Physical Chemistry (Practical)	SEC	0	0	4	2
9	XXX	Individualized Education Plan/ Tutorial*	0	0	4	0	0
Total				15	4	12	21

*Four non-credit hours (Four contact hours) for Individualized Education Plan/tutorial

DSC: Discipline Specific Core Course, **SEC:** Skill Enhancement Course, **AEC:** Ability Enhancement Course, **DSE:** Discipline Specific Elective Course, **IDC:** Interdisciplinary Course, **VAC:** Value Added Course.

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

Semester II							
S. No.	Course Code	Course Title	Course Type	L	T* **	P	Cr
1	MCHM.516	Chemistry of Clusters and Group Theory	DSC	3	0	0	3
2	MCHM.517	Organic Reagents and Photochemistry	DSC	3	0	0	3
3	MCHM.518	Molecular Spectroscopy and Statistical Thermodynamics	DSC	3	0	0	3
4	MCHM.409	Concepts in Chemistry	AEC	3	0	0	3
5	MCHM.519	Computational and Structural Chemistry (Practical)	SEC	0	0	4	2
6	MCHM.520	Advanced Chemistry Practical	SEC	0	0	4	2
Opt Any One (01) Value Added Course							
7	MCHM.511	Bioinorganic and Biophysical Chemistry	VAC	2	0	0	2
8	MCHM.512	Protein Chemistry					
9	XXX	Individualized Education Plan/ Tutorial*	0	0	4	0	0
Opt Any One (01) Discipline Elective Courses/MOOC							
10.	MCHM.521	Advanced Organic Chemistry	DSE	3	0	0	3
11	MCHM.522	Chemistry of Natural Products	DSE	3	0	0	
12	MCHM.523	Green Chemistry	DSE	3	0	0	
13	MCHM.524	Inorganic Spectroscopy and Catalysis	DSE	3	0	0	
14	MCHM.525	Solid State Chemistry and Statistical Thermodynamics	DSE	3	0	0	
15	MCHM.526	Supramolecular Chemistry	DSE	3	0	0	
16	MCHM.527	Polymer Chemistry	DSE	3	0	0	
17	MCHM.528	Inorganic Photochemistry	DSE	3	0	0	
18	MCMC.404	Advanced Medicinal Chemistry-I	DSE	3	0	0	
19	MBCH.508	Biomolecules and Bioenergetics	DSE	3	0	0	
20	XXX.XXX	Interdisciplinary Course/MOOC#	IDC	2	0	0	2
Total Credit (Hours)				19	4	8	23

Interdisciplinary Course Offered by Department for other Departments							
21	MCHM.506	Basics Perspective in Inorganic Chemistry	IDC	2	0	0	2
22	MCHM.507	Introduction to Green Chemistry and Sustainability	IDC	2	0	0	2
23	MCHM.508	Chemistry of Nanomaterials and Fabrication	IDC	2	0	0	2
24	MCHM.509	General Laboratory Practices	IDC	2	0	0	2
25	MCHM.510	Chemistry of Drug Design and Synthesis	IDC	2	0	0	2

**Opt Any One Skill Based/Skill Enhancement Course/ MOOC/NPTEL Course/Project Work for Exit with Post-Graduate Diploma in Chemistry							
26	MCHM.529	Project Report	SEC	0	0	8	4
27	MCHM.530	Chemical Laboratory Techniques	SEC	4	0	0	4
28	MCHM.531	Intellectual Properties Rights	SEC	4	0	0	4
29	MCHM.532	Modern Instrumental Methods	SEC	4	0	0	4
MOOC Courses							
30	XXXX	Forensic Chemistry and Explosives	SEC	4	0	0	4
31	XXXX	Biomass Characterization	SEC	4	0	0	4
32	XXXX	Analytical Techniques	SEC	4	0	0	4
33	XXXX	Drugs of Abuse	SEC	4	0	0	4
NPTEL Courses							
34	XXXX	Analytical Chemistry	SEC	4	0	0	4
35	XXXX	Food Oils & Fat : Chemistry and Technology	SEC	4	0	0	4
36	XXXX	Organic Chemistry in Biology & Drug Development	SEC	4	0	0	4
37	XXXX	Transition Metal Organometallic Chemistry: Principles to Application	SEC	4	0	0	4
38	XXXX	Any other ongoing MOOC/NPTEL courses, may be taken by the student after approval from the department	SEC	4	0	0	4

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

*Four non-credit hours (Four contact hours) for Individualized Education Plan/tutorial

**These courses are offered for students opting to exit after one year under Multiple Entry-Exit Scheme and will be given a Post-Graduate Diploma in Chemistry.

DSC: Discipline Specific Core Course, **SEC:** Skill Enhancement Course, **AEC:** Ability Enhancement Course, **DSE:** Discipline Specific Elective Course, **IDC:** Interdisciplinary Course, **VAC:** Value Added Course.

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

During Summer vacations, students are encouraged to perform 4-6 weeks of Summer Internship/Industrial Training at reputed University/Institute/Industry etc. It will be a non-credit exercise for the skill development of the students.

<u>Semester-III</u>							
S. No.	Course Code	Course Title	Course Type	L	T	P	Cr
1	MCHM.599-1	Dissertation Part-I	SB	0	0	40	20
		Total		0	0	40	20

<u>Semester-IV</u>							
S. No.	Course Code	Course Title	Course Type	L	T	P	Cr
1	MCHM.599-2	Dissertation Part-II	SB	0	0	40	20
		Total		0	0	40	20

DSC: Discipline Specific Core Course, **SEC:** Skill Enhancement Course, **AEC:** Ability Enhancement Course, **DSE:** Discipline Specific Elective Course, **IDC:** Interdisciplinary Course, **VAC:** Value Added Course.

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

Examination pattern and evaluation for Masters' students

Formative Evaluation: Internal assessment shall be 25 marks using any two or more of the given methods: tests, open book examination, assignments, term paper, etc. The Mid-semester test shall be descriptive type of 25 marks including short answer and essay type. The number of questions and distribution of marks shall be decided by the teachers.

Summative Evaluation: The End semester examination (50 marks) with upto 100% descriptive type and upto 30% objective type shall be conducted at the end of the semester. The objective type shall include one-word/sentence answers, fill-in the blanks, MCQs', and matching. The descriptive type shall include short answer and essay type questions. The number of questions and distribution of marks shall be decided by the teachers. **Questions for exams and tests shall be designed to assess course learning outcomes along with focus on knowledge, understanding, application, analysis, synthesis, and evaluation.**

The evaluation for IDC, VAC and entrepreneurship, innovation and skill development courses shall include MST (50 marks) and ESE (50 marks). The pattern of examination for both MST and ESE shall be same as ESE described above for other courses.

Evaluation of dissertation proposal in the third semester shall include 50% weightage by supervisor and 50% by HoD and senior-most faculty of the department. The evaluation of dissertation in the fourth semester shall include 50 marks for continuous evaluation by the supervisor for regularity in work, mid-term evaluation, report of dissertation, presentation, and final viva-voce; 50 marks (50% weightage) by an external expert shall be based on report of dissertation (25 marks), presentation (10 marks), novelty/originality (5 marks) and final viva-voce (10 marks). The external expert may attend final viva-voce through offline or online, hybrid mode.

Examination pattern

Discipline Specific Core, Discipline Elective, and Compulsory Foundation Courses			IDC, VB, and Skill Based Courses	
	Marks	Evaluation	Marks	Evaluation
Internal Assessment	25	Various methods	-	-

Mid-semester test (MST)	25	Descriptive		50	Descriptive (upto 100%) Objective (upto 30%)
End-semester exam (ESE)	50	Descriptive (upto 100%) Objective (upto 30%)		50	Descriptive (upto 100%) Objective (upto 30%)
Dissertation Proposal (Third Semester)			Dissertation (Fourth Semester)		
	Marks	Evaluation		Marks	Evaluation
Supervisor	50	Dissertation proposal and presentation	Supervisor/ co-supervisor(s)	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	50	Report of dissertation (25), presentation (10), novelty/originality (5) and final viva-voce (10)

Marks for internship shall be given by the supervisor/internal mentor and external mentor.

Some Guidelines for Internal Assessment

1. The components/pattern of internal assessment/evaluation should be made clear to students during the semester.
2. The results of the internal assessment must be shown to the students.
3. The question papers and answers of internal assessment should be discussed in the class.
4. The internal assessment shall be transparent and student-friendly and free from personal bias or influence.

Course Title: Transition Metal Complexes and Reaction Mechanism

Paper Code: MCHM.401

Total Contact Hours: 45

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

CLO1: Interpret the reaction mechanism, formation constant and stability of the coordination complexes.

CLO2: Interpret the electronic properties.

CLO3: Interpret the magnetic properties.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mapping with CLOs
Unit-1 10 Hours	<p>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.</p> <p><i>Group Discussion among the students on the stability of metal complex formation.</i></p>	CLO1
Unit-2 10 Hours	<p>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.</p> <p><i>Demonstration of reactions mechanism of metal complexes.</i></p>	CLO1
Unit-3 15 Hours	<p>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 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,</p>	CLO2

	Orgel diagrams, Tanabe Sugano diagrams, spectrochemical series, band intensities, factors influencing band widths. <i>Classroom discussion on interpretation of LS coupling and various energy level diagrams through brainstorming.</i>	
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). <i>Hands-on experience of metal complexes for magnetic properties by using Gouy's Balance.</i>	CLO3

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 (2019). NY Research Press.
10. Close, D. Principles of Inorganic Chemistry (2019). Larsen and Keller Education.

Course Title: Reaction Mechanism and Stereochemistry

Paper Code: MCHM.402

Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

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

CLO1: Identify various methods and intermediate species involved while determining the mechanism of organic reactions.

CLO2: Examine the mechanistic and synthetic aspects of nucleophilic, electrophilic substitution and elimination reactions.

CLO3: Explore the implications of addition to carbon-carbon/heteroatom multiple bonds for the synthesis of various molecules.

CLO4: Interpret and predict the energetically favoured conformation of cyclic and acyclic compounds, chirality and reactivity.

Units/ hours	Content	Mapping with CLOs
Unit-1 11 Hours	<p>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.</p> <p>Reactive intermediates: Structure and reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzyne. Neighbouring group participation, classical and non-classical carbocations, phenonium ions and norbornyl system.</p> <p>Free radical reactions: Free radical substitution mechanism at an aromatic substrate, reactivity for aliphatic and aromatic substrates at a bridgehead, Reactivity in the attacking radicals, the effect of solvents on reactivity, auto-oxidation. Hunsdiecker Reaction, Coupling of Alkynes, Acyloin Condensation, Bu₃SnH promoted reaction, Coupling of alkynes and arylation of aromatic compounds by diazonium salts.</p> <p><i>Classroom discussion on various tools used for the determination of reaction mechanisms.</i></p> <p><i>Peer Discussion on stability of the intermediates in the presence of different substituents (electron-withdrawing and electron releasing).</i></p> <p><i>Brainstorming on identification of free radical quenching reagents and role of free radicals in daily life.</i></p>	CLO1

Unit-2	Substitution and Elimination Reactions	CLO2
11 Hours	<p>Aliphatic nucleophilic substitution reactions: S_N1, S_N2, S_Ni and SET mechanism. Energy profile diagram, nucleophilic substitution at an allylic, aliphatic and vinylic carbon, leaving group and reaction medium, ambident nucleophile, ion pair theory.</p> <p>Aromatic nucleophilic and electrophilic substitution reactions: The S_NAr, bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure. Aromatic electrophilic substitution: arenium ion mechanism, <i>ortho/para</i> ratio</p> <p>Elimination reactions: E_2, E_1 and E_{1cB} mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, leaving group and medium, mechanism and orientation in pyrolytic elimination.</p> <p><i>Demonstration of substitution reactions with the help of ball and stick models.</i></p> <p><i>Peer discussion on the role of substituents in electrophilic and nucleophilic substitution reaction.</i></p>	
Unit-3	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.	CLO3
11 Hours	<p>Addition to carbon-hetero multiple bonds: Structure and reactivity of carbonyl group towards nucleophilic addition. Arndt-Eistert synthesis. Mannich, Benzoin, Perkin and Michael addition, Robinson annulation.</p> <p><i>Peer discussion of the mechanism of nucleophilic additions to carbonyl, nitrile, thiocarbonyl, carboxylic acids, esters and amides.</i></p> <p><i>Mechanistic interpretation of C-C, C-N and C-O bond formation reactions through brainstorming.</i></p>	

Unit-4 12 Hours	<p>Stereochemistry: Chirality, projection formulae, configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, diastereoselectivity, D/L, R/S, E/Z and <i>cis/trans</i> configurational notations, 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, Asymmetric Synthesis. Determination of absolute configuration. 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.</p> <p><i>Demonstration of conformational and configurational analysis, projection formulae and topicity of the molecules with the help of ball and stick models.</i></p> <p><i>Ball and stick models of biphenyls, allenes and spiranes for chirality.</i></p>	CLO4
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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. Yadav, L. D. S., Singh, J., and Singh, J. (2021). *Organic Synthesis*, Pragati Prakashan, India.
3. Norman, R. O. C., and Coxon, J. M. (1993). *Principle of Organic Synthesis*, CRC Press; 3rd edition.
4. Smith, M. B., and March, J. (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*. John Wiley and Sons.
5. Ahluwalia, V. K., and Parashar, R. K. (2011). *Organic Reaction Mechanisms*. Narosa Publishing House (P) Ltd.
6. McMurry, J. (1996). *Organic Chemistry*, Brooks. Cole, New York, 657.
7. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.
8. Bansal R. K. (2010). *Organic Reaction Mechanism*. New Age International (P) Ltd.
9. Kalsi, P. S. (2010). *Organic Reactions and Their Mechanisms*. New Age International, New Delhi.
10. Lowry, T. H. and Richardson K. S. (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., New York.
11. Morrison, R.T. and Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India.
12. Mukherjee, S. M. and Singh, S. P. (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi.

13. Solomon, T.W.G, Fryhle, C. B. and Snyder, S. A. (2013). *Organic Chemistry*. John Wiley and Sons, Inc.
14. Sykes, P. A. (1997). *Guide Book to Mechanism in Organic Chemistry*, Prentice Hall.
15. 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.
16. Morisaki, K., Morimoto, H., Ohshima, T. Recent Progress on Catalytic Addition Reactions to *N*-Unsubstituted Imines, *ACS Catal.* 2020, 10, 12, 6924–6951.
17. Singh, M. S. (2014). *Reactive intermediates in organic chemistry: Structure, Mechanism, and Reactions*. John Wiley & Sons.

CUP Library E Resource:

18. Nag, A. (Ed.). (2018). *Asymmetric synthesis of drugs and natural products*. CRC Press.

Course Title: Quantum Chemistry

Paper Code: MCHM.403

Total Contact Hours: 45

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

- CLO1:** Interpret and solve the Schrodinger equation for various systems, particle in a boundary model, Electronic and Hamiltonian operators for molecules.
- CLO2:** Explain the quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
- CLO3:** Relate the Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle with the atomic and molecular phenomena.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mapping with CLOs
Unit 1 11 Hours	<p>Fundamental Background: Review of essential mathematical concepts required for quantum chemistry, Postulates of quantum mechanics, Eigen values and Eigen functions, operators, Schrodinger equation.</p> <p>Translational, Rotational and Vibrational Motions: - Free particle and particle in a box and its application, one-dimensional harmonic oscillator and rigid rotor, particle in a ring, particle on a sphere.</p> <p><i>Problem solving approach to determine Eigen values and Eigen function using corresponding operator and Schrodinger equation. Brainstorming on defining and solving Schrodinger equation for different systems like particle in a box, rigid rotator, simple harmonic oscillator.</i></p>	CLO1
Unit 2 11 Hours	<p>Angular Momentum: Ordinary angular momentum, generalized angular momentum, Eigen functions and Eigen values for angular momentum, Ladder operator, addition of angular momenta</p> <p>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.</p> <p><i>Understanding multi-electron atom quantum evaluation through peer discussion and brainstorming sessions</i></p>	CLO2
Unit 3 12 Hours	<p>Variation Methods: The variation theorem and its application, linear variation principle.</p> <p><i>Understand the principles of variation theorem and its application through examples</i></p>	CLO3

Unit 4 11 Hours	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 <i>Application of Variation method and its uses in 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</i>	CLO3
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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. Atkins, P., De Paula, J., and Keeler, J. (2018). *Atkins' Physical Chemistry*. Oxford University Press.
9. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2008). *Physical Chemistry*. Wiley-Interscience Publication.
10. Kapoor, K. L. (2011). *Text Book of Physical Chemistry*.3/5, Macmillan Publishers.
11. McQuarrie, D. A. and Simon, J. D. (2018). *Physical Chemistry: A Molecular Approach*. Viva Books.
12. Puri, B.R., Sharma, L.R. and Pathania, M.S. (2013). *Principles of Physical Chemistry*. Vishal Publishing Company.
13. Atkins, P., De Paula, J. and Keeler, J. (2018). *Atkins' Physical Chemistry*. 11th ed. Oxford University Press.

Course Title: Spectroscopic Techniques

Paper Code: MCHM.404

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

- CLO1:** Explore various spectroscopic techniques (UV, IR, NMR and MS) used in organic synthesis for structure elucidation.
- CLO2:** Predict NMR spectra and various fragment-ions/peaks in MS of a given molecular structure.
- CLO3:** Analyze and interpret the combined spectroscopic data (UV-Vis, IR, ^1H & ^{13}C NMR) for structural elucidation of unknown organic molecules.

Units/ Hours	Content	Mapping with CLOs
Unit-1 11 Hours	<p>UV-Visible spectroscopy: Introduction, role of solvents, chromophores and their interaction with UV-visible radiation. Woodward-Fieser rule for conjugated dienes and carbonyl compounds.</p> <p>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.</p> <p><i>Problem solving - Identification of the structure from the given UV and FTIR data.</i></p>	CLO1
Unit-2 12 Hours	<p>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.</p> <p><i>The role of external magnetic field on precessional frequency: Peer discussion.</i></p>	CLO1, CLO2
Unit-3 11 Hours	<p>^{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 (^1H-^1H COSY), Hetero COSY (^1H-^{13}C COSY, HMQC), long range ^1H-^{13}C COSY (HMBC), NOESY.</p> <p><i>Problem solving - Identification of the structure from the given ^1H and ^{13}C NMR data.</i></p>	CLO1, CLO2, CLO3

Unit-4 11 Hours	<p>Mass spectrometry: Basic principles and brief outline of instrumentation. Ion formation: EI, CI, FAB, MALDI, ESI, metastable ion, alpha-cleavage, McLafferty rearrangement, Retro-Diels-Alder cleavage, nitrogen rule, fragmentation process of organic molecules in relation to molecular structure determination. Relative abundance of isotopes.</p> <p>Hyphenated Techniques: GC-MS, LC-MS. High resolution mass spectrometry (HRMS).</p> <p><i>Problems Solving for structure elucidation using the above spectroscopic techniques.</i></p> <p><i>Interpretation of various fragmentation peaks in the mass spectrum of the given sample.</i></p>	CLO1, CLO2, CLO3
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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. Kalsi, P. S. (2007). *Spectroscopy of Organic Compounds*. New Age International.
5. Kemp, W. (2019, 2nd edition). *Organic Spectroscopy*, ELBS. MACMILLAN.
6. Melinda, J.D. (2010). *Introduction to Solid NMR Spectroscopy*. Wiley India Pvt Ltd.
7. Silverstein, R. M., Webster, F. X., Kiemle, D. J., and Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John Wiley and sons.
8. Pretsch, E., Bühlmann, P., Badertscher, M. (2020). *Structure Determination of Organic Compounds*. Springer-Verlag Berlin Heidelberg.
9. Price, W. S. (2024). *Annual reports on NMR spectroscopy* (Vol. 111). Elsevier.

Course Title: Thermodynamics, Kinetics and Electrochemistry

Paper Code: MCHM.405

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

CLO1: Predict the thermodynamic of mixtures, solutions and phase transformations.

CLO2: Establish and evaluate the mechanism and kinetics for reactions.

CLO3: Interpret the fast reaction monitoring for complex reactions.

CLO4: Evaluate and predict the spontaneity of a redox processes in electrochemical systems.

CLO5: Apply activity coefficient calculated of solution using Debye-Huckel theory and Ideally-Dilute solutions in chemical aspects.

CLO6: Predict and establish the thermodynamic and kinetic aspects of adsorption and catalysis.

Units/ Hours	Content	Mapping with CLOs
Unit 1 12 Hours	<p>Classical Thermodynamics and Phase Transitions: Introduction to thermodynamics, Thermodynamics of mixing, Partial Molar Properties, Gibbs- Duhem equation, Chemical potential of liquids and solutions, Phase transition: Clausius-Clapeyron equation.</p> <p>Reaction Kinetics: Introduction, complex reactions, steady state approximation, kinetic mechanisms of chemical reactions, Arrhenius and Eyring equations and their applications, collision theories of rate constant, treatment of unimolecular reactions, steric factor, ionic reactions: salt effect.</p> <p><i>Understanding chemical kinetics and potential surface-reaction coordinate by hands-on activity either as gaming, stochastic or molecular dynamic models</i></p>	CLO1, CLO2
Unit 2 11 Hours	<p>Photochemical Reactions and Processes: Laws of photochemistry and kinetics of photochemical reactions.</p> <p>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 and its application in chemistry and biology.</p> <p><i>Learning photochemical reaction kinetics through problem solving activities. Understanding the ultrafast kinetic process and its application through examples.</i></p>	CLO2, CLO3
Unit 3 11 Hours	<p>Electrochemistry: Activity, Activity coefficient; determination of activity and activity coefficients, Activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions.</p> <p>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.</p> <p><i>Understanding application of electrochemistry using classroom games activity. Expanding the understanding of conductance application using peer learning.</i></p>	CLO4, CLO5

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, application of enzyme catalysis. <i>Application and challenges in adsorption towards environmental and nanomaterial through peer learning. Enzyme binding and catalysis through inquiry guided and gaming based learning.</i>	CLO2, CLO6
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Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming

Suggested Readings

- Engel, T., Reid, P. and Hehre, W. (2012) *Physical Chemistry*. Pearson Education
- Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company Nash,
- Nelson, K. A., Bawendi, M. (2008) <https://ocw.mit.edu/courses/chemistry/5-60-thermodynamics-kinetics-spring-2008/video-lectures>.
- 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
- 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
- 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
- Drennan, C., Taylor, E. V., (2008) <https://ocw.mit.edu/courses/chemistry/5-111-principles-of-chemical-science-fall-2008/index.htm>
- Griffin, R. G., Voorhis, T. V. (2007) <https://ocw.mit.edu/courses/chemistry/5-111-principles-of-chemical-science-fall-2008/index.htm>
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- Laidler, K. J. (2003). *Chemical Kinetics*. Pearson Education Ltd.
- Atkins, P., De Paula, J., and Keeler, J. (2018). *Atkins' Physical Chemistry*. Oxford University Press.
- Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2008). *Physical Chemistry*. Wiley-Interscience Publication.
- Engel, T. and Reid, P. (2012). *Thermodynamics, Statistical Thermodynamics, and Kinetics*. Pearson Education.
- Lakowicz, J. R. (2006). *Principles of Fluorescence Spectroscopy*. Springer.
- Kapoor, K. L. (2011). *Text Book of Physical Chemistry*. 3/5, Macmillan Publishers.

16. McQuarrie, D. A. and Simon, J. D. (2018). *Physical Chemistry: A Molecular Approach*. Viva Books.
17. Moore, J. W., and Pearson, R. G. (1981). *Kinetics and Mechanism*. John Wiley and Sons.
18. Puri, B.R., Sharma, L.R. and Pathania, M.S. (2013). *Principles of Physical Chemistry*. Vishal Publishing Company.
19. 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.
20. 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.
21. 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.
22. Atkins, P., De Paula, J. and Keeler, J. (2018). *Atkins' Physical Chemistry. 11th ed.* Oxford University Press.

Course Title: Inorganic Chemistry (Practical)

Paper Code: MCHM.406

Total Contact Hours: 60

Learning Outcome: The students will be able to

CLO1: Perform volumetric and gravimetric analysis of cations and anions within reaction mixtures.

CLO2: Standardize and titrate various inorganic compounds.

L	T	P	Cr
0	0	4	2

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 $\text{C}_2\text{O}_4^{2-}$ ions.
3. Standardization of $\text{K}_2\text{Cr}_2\text{O}_7$ with Fe^{2+} and determination of Fe^{3+} (Ferric alum)
4. Standardization of hypo solution with potassium iodate / $\text{K}_2\text{Cr}_2\text{O}_7$ 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.

Course Title: Organic Chemistry (Practical)

Paper Code: MCHM.407

Total Contact Hours: 60

L	T	P	Cr
0	0	4	2

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

CLO1: Exercise good laboratory practices including safe handling of hazardous chemicals, laboratory glassware and equipment(s).

CLO2: Apply various experimental skills for purification, isolation and recrystallization of organic molecules.

CLO3: Analyze the progress of a given reaction with various chromatographic techniques.

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 reactions 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.

Course Title: Physical Chemistry (Practical)

Paper Code: MCHM.408

Total Contact Hours: 60

Learning Outcome: The students will be able to

CLO1: Develop skills on titrimetric analysis using conductivity meter, potentiometer and pH meter as well as buffer preparation and use.

CLO2: Hands on skills in viscometer, refractometer and spectrophotometer for different applications.

L	T	P	Cr
0	0	4	2

Experiments:

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 $\text{Fe}^{2+}/\text{Fe}^{3+}$ system by potentiometer using potassiumpermanganate
4. Preparation of buffers and measurement of their pH.
5. Determination of stability constant for Cu(II)-glycinate complex using potentiometry.
6. Determination of pK_a of acetic acid and H_3PO_4 by potentiometric titration using NaOH.
7. Determination of Surface tension of a given liquid.
8. Determination of refractive indices (RI) of given liquids and determination of the concentration from RI.
9. Verification of the Lambert-Beer's law and determination of extinction coefficient
10. Determination of stability constant of Fe(III)-salicylic acid complex by spectrophotometer.
11. To verify Freundlich and Langmuir adsorption isotherms for adsorption of acetic acid on activated charcoal.
12. Determination of partition coefficient of iodine between water and octanol and determination of equilibrium constant of tri-iodide.
13. Determination of rate constant and energy of activation of hydrolysis of an ester
14. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine-clock reaction.
15. Determination of thermal stability of biomacromolecules.
16. Determination of rate constant and energy of activation of a chemical reaction by visible and fluorescence spectroscopy.

Mode of Transactions: Demonstration, Experimentation, handling 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. Chand and 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.

Course Title: Chemistry of Clusters and Group Theory

Paper Code: MCHM.516

Total Contact Hours: 45

Learning Outcome: The students will able to interpret

CLO1: Concepts to realize point group within chemical structure, character tables and projection operator techniques.

CLO2: Application of symmetry and group theory in spectroscopy.

CLO3: Structural properties of organometallic complexes and their uses.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mapping with CLOs
Unit-1 10 Hours	<p>Symmetry: Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination.</p> <p><i>Basic discussion about types of symmetry and parameters to decide point groups in different molecules using of ball and stick models</i></p>	CLO1
Unit-2 10 Hours	<p>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.</p> <p><i>Group discussion to design the character tables of taking molecular examples and implication of ball and stick model tools.</i></p>	CLO2

Unit-3 15 Hours	<p>Metal Complexes: Organic-transition metal chemistry, complexes with π-acceptor and π-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.</p> <p><i>Discussion of various electron count rules and structural bonding parameters of organometallic compounds.</i></p>	CLO3
Unit-4 10 Hours	<p>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.</p> <p>Cage compounds of boron: boron cage compounds, boranes, carboranes and metallocene carboranes.</p> <p><i>Peer discussion on Cage clusters formation rules via Wede`s and Mingos rules.</i></p>	CLO4

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 (2019). NY Research Press.
9. Close, D. Principles of Inorganic Chemistry (2019). Larsen and Keller Education.

Course Title: Organic Reagents and Photochemistry

Paper Code: MCHM.517

Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcome: The students will be able to

CLO1: Interpret and predict the product formation of various photochemical reactions.

CLO2: Differentiate between thermally and photochemically driven pericyclic reactions and explain about their stereochemical aspects.

CLO3: Apply various oxidizing and reducing reagents in a logical manner for their application in functional group transformation in organic synthesis.

CLO4: Explore various molecular rearrangements and name reactions for the conversion of different functional groups.

Units/ hours	Content	Mapping with CLOs
Unit-1 11 Hours	<p>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, Ene/Alder-ene reaction, Hofmann-Löffler Fretag.</p> <p>Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Barton Nitrite Photolysis Reaction, Barton Decarboxylation, Singlet molecular oxygen reactions.</p> <p><i>Application of photochemical reactions in biologically important molecules through peer learning.</i></p> <p><i>Primary and secondary processes of photochemical reactions of carbonyl compounds and alkenes.</i></p>	CLO1
Unit-2 11 Hours	<p>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.</p> <p>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.</p> <p>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. 1-3-dipolar cycloaddition reaction (Huisgen reaction).</p> <p>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.</p> <p><i>Group project on the symmetry elements in FMO of $4n\pi$ and $(4n+2)\pi$ electrons containing substrates.</i></p> <p><i>Quiz on FMO, correlation diagram and PMO approaches for pericyclic reactions.</i></p>	CLO2

Unit-3 12 Hours	<p>Oxidizing and Reducing Reagents: Mechanism, selectivity, stereochemistry and applications of oxidation reactions, oxidation reactions using DDQ, NBS, Pb(OAc)₄, SeO₂, PCC, PDC, Cr and Mn based reagents, Periodic acid, OsO₄, Swern oxidation, Hydroboration-oxidation, epoxidation using peracids. Baeyer-Villiger oxidation, Sharpless epoxidation, Oppenauer oxidation.</p> <p>Reducing Agents: Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts (Lindlar, Rosenmund, Adam's catalysts), Wilkinson's catalyst, Meerwein-Ponndorf-Verley reduction, dissolving metal reductions, Birch reduction, Reductions using metal hydride NaBH₄, Luche reduction, NaBH₃CN, L-selectride, K-selectride, NaBH(OAc)₃, LiAlH₄, DIBAL-H, Diimide reduction.</p> <p><i>Peer discussion on selective use and careful handling of reducing agents.</i></p> <p><i>Demonstration on the synthesis and application of oxidizing agents like PCC. Peer discussion on green oxidizing agents.</i></p>	CLO3
Unit-4 11 Hours	<p>Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzilic acid, Favorskii, Neber, Beckmann, Hofmann, Curtius, Lossen, Schmidt, Carroll, Gabriel-Colman, Smiles and Sommelet-Hauser rearrangements. Dakin reaction.</p> <p>New synthetic reactions: Baylis-Hillman reaction, Biginelli reaction, Mitsunobu reaction, Buchwald-Hartwig coupling, Eishenmosher-Tanabe fragmentation, Shapiro reaction, Stork-enamine reaction, Vilsmeier-Haack reaction.</p> <p><i>Predicting the mechanistic pathways of rearrangement reactions through peer discussion.</i></p> <p><i>Application of important name reactions for bioactive molecule synthesis through brainstorming.</i></p>	CLO4

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.

Course Title: Molecular Spectroscopy

Paper Code: MCHM.518

Total Contact Hours: 45

Learning Outcome: The students will be able to

- CLO1:** Apply microwave, infrared-vibration-rotation Raman and infra-red Spectroscopy for chemical analysis and prediction of molecular structure
- CLO2:** Demonstrate and apply electronic absorption and emission spectroscopy of elements and simple molecules.
- CLO3:** Demonstrate and elucidate the physical principles of nuclear magnetic and electron spin resonance spectroscopy.
- CLO4:** Explore application of laser spectroscopy and photoelectron spectroscopy in materials and biomaterials.

L	T	P	Cr
3	0	0	3

Units/ Hours	Content	Mapping with CLOs
Unit 1 12 Hours	<p>Electronic Spectroscopy: Electronic transition, energy of electronic transition, selection rules, the Franck-Condon principle. UV-Visible and CD spectroscopy</p> <p>Photoluminescence: Jablonski Diagram; Measurement of fluorescence and phosphorescence lifetimes, photosensitization, quenching and photodimerization, Stern-Volmer equation.</p> <p>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.</p> <p><i>Problem solving approach to determine the bond length of diatomic and polyatomic molecules and effect of isotopic substitution on transition frequencies.</i></p>	CLO1, CLO2
Unit 2 11 Hours	<p>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.</p> <p>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.</p> <p><i>Brainstorming on use of electronic, pure vibrational, pure rotational and vibrational-rotational spectroscopy in understanding chemical characteristics.</i></p>	CLO3

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. <i>Understanding applications of magnetic resonance spectroscopy through peer learning and brainstorming.</i>	CLO4
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, X-ray photoelectron spectroscopy XPS. Application of XPS. <i>Understanding application and instrumentation of laser, photoelectron and atomic force spectroscopy through peer discussion.</i>	CLO5, CLO6

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

Suggested Readings

- Hollas, J. M. (2004). *Modern Spectroscopy*. John Wiley and Sons.
- Lakowicz, J. R. (2006). *Principles of Fluorescence Spectroscopy*. Springer.
- Barrow, G. M. (2007) *Physical Chemistry*. Tata McGraw-Hill Publishers.
- Banwell, C. N., and McCash, E. M. (1994). *Fundamentals of Molecular Spectroscopy* (Vol. 851). New York: McGraw-Hill.
- Carrington, A., and McLachlan, A. D. (1967). *Introduction to Magnetic Resonance: With Applications to Chemistry and Chemical Physics*. Chapman and Hall, London.
- Lynden-Bell, R. M., and Harris, R. K. (1969). *Nuclear Magnetic Resonance Spectroscopy*. Appleton-Century-Crofts.
- Reilley, C. N., Everhart, D. S., and Ho, F. F. L. (1982). *Applied Electron Spectroscopy for Chemical Analysis*. *Chemical Analysis*, 63, 105. John Wiley.
- Chang, R. (1971). *Basic Principles of Spectroscopy*. McGraw-Hill.
- Ghosh, P. K. (1983). *Introduction to Photoelectron Spectroscopy*. John Wiley and Sons, New York.
- Günther, H. (2013). *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*. John Wiley and Sons.
- Atkins' P. (2014) *Physical Chemistry*, Peter Atkins and Julio Paula, Oxford University Press; 10th Ed.
- 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
15. McQuarrie, D. A. and Simon, J. D. (2019) *Physical Chemistry: A Molecular Approach*. Viva Books
16. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2004) *Physical Chemistry*. Wiley-Interscience Publication.

Course Title: Concepts in Chemistry

Paper Code: MCHM.409

Total Contact Hours: 60

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

CLO1: Identify various retrosynthetic strategies and design the synthesis of target molecules.

CLO2: Apply the concepts of chemistry for controlling the selectivity of various organic transformations.

CLO3: Design various processes for the synthesis of commercially important molecules taking into consideration the protection and deprotection strategies.

CLO4: Know the aspects of structural and bonding of ionic, covalent and coordination molecules and compounds.

CLO5: Elucidate the aspects of s, p, d and f-block elements.

CLO6: Physical concept involving quantities errors, Kinetics, Thermodynamics, photochemistry and electrochemistry.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mapping with CLOs
Unit-1 11 Hours	<p>Functional group interconversion (FGI), retrosynthetic analysis involving chemoselectivity and regioselectivity. Use of acetylene and aliphatic nitro compounds in organic synthesis. Reversal of polarity (umpolung). C-X and C-C disconnections, amine synthesis. Protection and deprotection of various functional groups. Mechanism of naming reactions, transformations and reagents in organic synthesis.</p> <p><i>Brainstorming on identification of the retrosynthetic route of some recently FDA approved commercial drug molecules.</i></p> <p><i>Demonstration on the role of protecting groups in synthesis of commercial drugs.</i></p> <p><i>Problem solving based on NET-GATE Examination.</i></p>	CLO1
Unit-2 11 Hours	<p><i>Asymmetric synthesis, enantiomeric excess, stereo and regioselectivity. Organic transformations based on photochemical and concerted mechanisms.</i></p> <p><i>Combined problems on NMR, IR, Mass and UV.</i></p> <p><i>Problems based on photochemistry and pericyclic chemistry.</i></p> <p><i>Problem solving based on NET-GATE Examination.</i></p>	CLO2
Unit-3 11 Hours	<p>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 pKa, HSAB concept, Buffer solution. Properties of solid state and solution phase, reaction mechanism in metal compounds, cluster chemistry, Inorganic spectroscopy.</p> <p>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.</p> <p><i>Problem solving based on NET-GATE Examination.</i></p>	CLO3

Unit-4 12 Hours	<p>Thermodynamics: Concepts involved in first, second and third law of thermodynamics, Maxwell relations, Helmholtz and Gibbs Energies, equilibrium constant, temperature-dependence of equilibrium constant and Van't Hoff equation, Colligative properties of solutions.</p> <p>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.</p> <p>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.</p> <p><i>Problem solving based on NET-GATE Examination.</i></p>	CLO4
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Mode of Transactions: Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brainstorming.

Suggested Readings

1. Yadav, L. D. S., Singh, J., and Singh, J. (2017). Organic Synthesis, Pragati Prakashan, India.
2. Warren, S., and Wyatt, P., (2010). Designing Organic Synthesis: A Disconnection Approach. John Wiley and Sons.
3. Smith, M. B., (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*. John Wiley and Sons.
4. Carruthers, W. (2004). *Some Modern Methods of Organic Synthesis*. Cambridge Uni. Press, UK.
5. Li, J. J., (2014). *Name Reactions: A Collection of Detailed Reaction Mechanism*. Springer-Verlag.
6. Kalsi, P. S. (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 2: Stereochemistry and the Chemistry of Natural Products*. Pearson Education, UK.
8. Fleming I., (2011). *Molecular Orbitals and Organic Chemical Reactions*. John Wiley and Sons.
9. McMurry, J. (1996). *Organic Chemistry*, Brooks Cole.
10. Mukherjee, S. M., and Singh, S. P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd.
11. Solomon, T. W. G., Fryhle, C. B. and Snyder, S. A., (2013). *Organic Chemistry*. John Wiley and Sons, Inc.
12. Sykes, P. A. (1997). *Guide Book to Mechanism in Organic Chemistry*. Prentice Hall.
13. 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

14. Schettini, R., & Della Sala, G. (2021). New Trends in Asymmetric Catalysis. *Catalysts*, 2021, 11, 306.
15. 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.
16. 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.
17. Cotton, F. A., and Wilkinson, G. (1988). *Advanced Inorganic Chemistry* (Vol. 545). New York: Wiley.
18. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
19. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
20. Miessler, G. L. and Tarr, D. A. (2011). *Inorganic Chemistry*, Pearson Education.
21. Atkins, P. (2010). *Shriver and Atkins' Inorganic Chemistry*. Oxford University Press, USA.
22. Barrow, G. M. (2007). *Physical Chemistry*. Tata McGraw-Hill Publishers.
23. Kapoor, K. L. (2011). *Text Book of Physical Chemistry*. 3/5, Macmillan Publishers.
24. Atkins, P. and De Paula, J. (2009). *Atkins' Physical Chemistry*. Oxford University Press.
25. Moore, J. W. and Pearson, R. G. (1981). *Kinetics and Mechanism*. John Wiley and Sons.
26. Puri, B. R., Sharma L.R. and Pathania, M. S. (2013). *Principles of Physical Chemistry*. Vishal Publishing Company.
27. Laidler, K. J. (1987). *Chemical Kinetics*. Pearson Education Ltd. 50.
28. Rohatgi-Mukherjee, K. K., (1986). *Fundamentals of Photochemistry*. New Age International.
29. 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.
30. Gulevich, A. V., Dudnik, A. S., Chernyak, N., and Gevorgyan, V., Transition Metal Mediated Synthesis of Monocyclic Aromatic Heterocycles. *Chem. Rev.* 2013, 113, 3084-3213.

Course Title: Computational and Structural Chemistry (Practical)

Paper Code: MCHM.519

L	T	P	Cr
0	0	4	2

Total Contact Hours: 60

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

CLO1: Use and get skilled in a variety of chemistry software needed for higher studies.

CLO2: Elucidate the structure of unknown compounds via spectral interpretation of ^1H , ^{13}C NMR, IR, UV and Mass spectrum.

CLO3: Select and apply the data analytics to every process and analysis in chemistry, thereby bringing in quality control to his work in hand.

Experiments:

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

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

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

Spectral interpretation: Interpretation of UV, IR, NMR (1D & 2D-NMR) and mass spectrum.

Combined Structure problems: Exercises of structure elucidation of unknown compounds via combined spectral interpretation of IR, UV-Visible, ^1H and ^{13}C NMR and mass spectra, along with two-dimensional NMR spectroscopy.

Statistical Analysis Methods:

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 spectrometers.
5. Non-Linear least square fitting for adsorption and kinetic data.
6. Determination of ANOVA for intra-laboratory testing.
7. Error function and residual analysis of Linear and Non-linear least square fitting
8. Optimization of process and analysis using Factor analysis, Principal 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.

- Pasto, D.P., Johnson, C., Miller, M. (2010). Experiments and Techniques in Organic Chemistry, Prentice Hall.
- Vogel, A.I. (2003). Text Book of Practical Organic Chemistry, Pearson.
- Armarego, W. L., & Chai, C. (2012). Purification of Laboratory Chemicals. Butterworth-Heinemann.
- Findeisen, M., (2013). 50 And More Essential NMR Experiments: A Detailed Guide. John Wiley & Sons.
- 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.
- Yorck, M.M., and Neuhold, M., (2007). Practical Data Analysis in Chemistry, 26, Elsevier Science.
- https://www.practicaldatascience.org/html/pandas_series.html.
- Leszczynski, J., Shukla, M. (2012). Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends, Springer Netherlands.

Course Title: Advanced Chemistry Practical

Paper Code: MCHM.520

Total Contact Hours: 60

L	T	P	Cr
0	0	4	2

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

CLO1: Identify various reagents used for drying of solvents and their disposal.

CLO2: Separate and purify the desired product from an organic reaction mixture.

CLO3: Characterize organic compounds using various spectroscopic techniques.

CLO4: Realize the impact of various coupling and click chemistry strategies for construction of value added chemicals.

CLO5: Perform 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 P₂O₅ and safe disposal of residual P₂O₅.

- Synthesis:** Separation and purification of organic compounds by column chromatography, percentage yield calculation (any seven):
 - 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-Vinylguaiaicol.
 - To study Buchwald-Hartwig reaction of aryl halide with an amine using Cu-based catalyst.
 - Synthesis of triazole *via* reaction of alkyne 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 benzo-fused heterocyclic compounds
 - 3-Acetyl coumarin
 - Benzothiazole
 - Pyrazole
 - Isoxazole
 - 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

13. To study the Vielsmeyer-Haack reaction of indole/acetophenones.
14. To study the three component coupling for the synthesis of (any one)
 - a. dihydropyrimidinone (*via* Biginelli reaction)
 - b. propargylamine (*via* A^3 -coupling)
2. **Advanced Instrumentation Experiments:**
 1. Determination of concentrations of proteins and DNA using spectrophotometer
 2. Structural analysis of amino acids and proteins using CD, NMR and Fluorescence spectrometers.
 3. Study of thermal denaturation (T_m and DH_m) of proteins and DNA using UV-Visible spectrophotometer, CD spectrometer and DSC.
 4. Measurement of zeta potential and sizes of nanoparticles by DLS.
 5. Determination of Michaelis-Menten (K_m) constant in enzyme kinetics.
 6. Particle size and hydrodynamic radii analysis for adsorbents, protein or nanoparticles.
 7. 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 A^3 -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 Hilde, K.E., Johnson W.C. and Ho John, P.S. (2005). *Principles of Physical Biochemistry* 2nd 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: Bioinorganic and Biophysical Chemistry

Paper Code: MCHM.511

L	T	P	Cr
2	0	0	2

Total Contact Hours: 30

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

CLO1: Determine structure and biological functions of metalloproteins and enzymes.

CLO2: Classify metallobiomolecules on the basis of their functional properties.

CLO3: Analyze the role of metal ions in the biological system.

CLO4: Determine the factors that govern the thermodynamic and mechanical stability, folding, and dynamics of proteins.

CLO5: Interpret kinetics, thermodynamics, and mechanism of protein folding.

Units/ hours	Content	Mappin g with CLOs
Unit 1 7 Hours	<p>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.</p> <p><i>Brainstorming regarding structure-function relationship of heme and non-heme protein.</i></p>	CLO1
Unit 2 8 Hours	<p>Inorganic Chemistry of Enzymes – II: Metallothioneins: Ferredoxins, carboxypeptidase, carbonic anhydrase, blue copper proteins, superoxide dismutase and hemocyanins.</p> <p>Enzymes: Structure and function, inhibition and poisoning vitamin B₁₂ and B₁₂ coenzymes metallothioneins, bio-inorganic chemistry of Mo and W.</p> <p><i>Comparison of the reactivity of Ferredoxins and artificial Iron-sulfur clusters.</i></p> <p><i>Peer group discussion on structure-function relationship of metallothioneins and metalloenzymes.</i></p>	CLO2
Unit 3 8 Hours	<p>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.</p> <p><i>Group discussion on the significance of metal ions and non-metals in various diseases.</i></p>	CLO3

Unit 4 7 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. <i>Demonstration of applications of spectroscopic and calorimetric techniques for biochemical and biophysical characterizations of macromolecules.</i>	CLO4, CLO5
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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., Overton, T., Rourke, J., Weller, J., and Armstrong, F., (2010). *Shriver and Atkins' Inorganic Chemistry*. Oxford University Press.
6. Cowan, J. A. (1997). *Inorganic Biochemistry: An Introduction*. Wiley – VCH.
7. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vol. 18, Wiley-Interscience.
8. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vol. 38, Wiley-Interscience.
9. Lesk, A. M., (2010). *Introduction to Protein Science: Architecture, Function, and Genomics*. Oxford University Press.
10. Cantor, C. R. and Schimmel, P. R., (1980). *Biophysical Chemistry*. Freeman.
11. Van Holde, K. E., Johnson, W.C., and Ho, P. S., (2006). *Principles of Physical Biochemistry*. Pearson Education.
12. Harding, S. E. and Chowdhry, B. Z. (2001). *Protein-Ligand Interactions*. Oxford University Press.
13. Kepp, K. P., Bioinorganic Chemistry of Alzheimer's Disease. *Chem. Rev.* 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. *Chem. Rev.* 2018, 118, 2718-2768.
15. Huang, X., and Groves, J. T., Oxygen Activation and Radical Transformations in Heme Proteins and Metalloporphyrins. *Chem. Rev.* 2018, 118, 2491-2553.

Value Added Course (VAC)

Course Title: Protein Chemistry

Paper Code: MCHM.512

Total Contact Hours: 30

Learning Outcome: The students will be able to interpret and analyze

CLO1: Structure and biological functions of proteins.

CLO2: The role of metals in biology

CLO3: Mechanism of protein folding

CLO4: The cause and treatment of neurodegenerative, iron metabolic disorder and diabetes.

L	T	P	Cr
2	0	0	2

Units/ hours	Content	Mapping with CLOs
Unit-1 8 Hours	Buffers; Amino Acids; Proteins: Function and Structure, Protein synthesis; Protein engineering and protein/protein interactions. <i>Group discussion regarding in-vivo and in vitro protein folding.</i>	CLO1
Unit-2 7 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. <i>Brainstorming regarding the role of metals in health and diseases and interlink between iron metabolic disorder and diabetes.</i>	CLO2
Unit-3 7 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; <i>Peer group discussion on understanding how protein folds/misfolds and forms amyloid fibrillation and their treatment and diagnosis.</i>	CLO3
Unit-4 8 Hours	Practical implications in biotechnology; Special emphasis on human protein deposition diseases including Alzheimer's, Parkinson's and Huntington's disease. <i>Demonstration of role of chaperones and peptides on preventing amyloid fibril formation in human natively disordered proteins.</i>	CLO4

Mode of Transactions: Demonstration, Experimentation, handling 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., Overton, 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: Advanced Organic Chemistry

Paper Code: MCHM.521

Total Contact Hours: 45

Learning Outcome: The students will be able to

CLO1: Compare the reactivity of smaller, five and six membered heterocyclic compounds.

CLO2: Explore various reagents for functional group conversions and synthesis of organic frameworks.

CLO3: Design the synthesis of alkenes and functionalized molecules utilizing phosphorus, nitrogen and sulphur ylides.

CLO4: Apply various cross-coupling reactions and organoborane based reagents for the synthesis of fine-chemicals.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mappin g with CLOs
Unit-1 11 Hours	<p>Heterocyclic Chemistry: Systematic (Hantzsch-Widman system) and replacement nomenclature for monocyclic, fused and bridged heterocycles.</p> <p>Three-membered and four-membered heterocycles: aziridines, oxiranes, thiranes, azetidines, oxetanes.</p> <p>Five membered heterocycles containing two heteroatoms (S, N, O): Diazoles (imidazole, pyrazole), triazoles, oxazoles and thiazoles.</p> <p>Six-membered heterocycles: Synthesis and reactions of coumarins, chromones.</p> <p>Benzo-fused five-membered heterocycles: Indoles, benzofurans and benzimidazoles.</p> <p><i>Debate on reactivity order, basic and aromatic character of five- and six- membered heterocycles containing one and two heteroatoms.</i></p>	CLO1
Unit-2 11 Hours	<p>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, Lawesson reagent, IBX, Fetizon reagent, Dioxiranes, Tebbe reagent, Corey-Nicolaou reagent and macrolactonization, Mosher's reagent.</p> <p><i>Comparison of the reactivity and selectivity of various reagents through collaborative learning.</i></p>	CLO2

Unit-3 11 Hours	<p>Reaction of ylides: Phosphorus ylide; structure and reactivity, stabilized ylides, Wittig, Wittig-Horner and Wadsworth Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification. Sulphur ylides; stabilized and non-stabilized ylides. Nitrogen Ylides; Stevens rearrangement, Sommelet-Hauser rearrangement. Wittig vs Peterson's olefination.</p> <p>Enolate Chemistry: Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, counter-cation and electrophiles; thermodynamically and kinetically controlled enolate formations; various transition state models to explain stereoselective enolate formation; enamines and metallo-enamines; regioselectivity in generation.</p> <p><i>Peer group discussion on various methods to construct double bonds (including exocyclic double bonds) and respective advantages.</i></p> <p><i>Group discussion on stereoselective generation of enolates and alkylation in organic synthesis.</i></p>	CLO3
Unit-4 12 Hours	<p>Organometallic compounds: Organoboranes: Preparation of organoboranes with $\text{BH}_3\text{-THF}$, dicyclohexylborane, disiamylborane, thexylborane, 9-BBN. Functional group transformations of organoboranes: oxidation, protonolysis and rearrangements, formation of carbon-carbon-bonds viz organoboranes carbonylation. Chiral Organoboranes: diisopinocampheyl borane, alpine borane.</p> <p>Cross-Coupling C-C and C-N coupling reactions: Heck coupling, Sonogashira coupling, Suzuki coupling, Buchwald Coupling, Negishi coupling, Chan-Lam coupling.</p> <p><i>Expression of the views of the students on latest advancement in the area of organoboranes including stereochemical aspects through presentation.</i></p>	CLO3, CLO4

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

Suggested Readings

1. Yadav, L. D. S., Singh, J., and Singh, J. (2017). *Organic Synthesis*, Pragati Prakashan, India.
2. Norman, R.O.C., and Coxon, J. M. (1993). *Principle of Organic Synthesis*, CRC Press; 3rd edition.
3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*. Narosa Publishing House (P) Ltd., New Delhi.
4. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John Wiley and Sons.
5. Carey, F. A., and Sundberg, R. J. (2007). *Advanced organic chemistry: part B*. Springer Science and Business Media.
6. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.

7. Bansal, R. K. *Heterocyclic Chemistry*, 5th Edition, 2010. New Age International (P) Ltd., New Delhi.
8. Gilchrist, T. L., (1997). *Heterocyclic Chemistry*. Addison Wesley Longman Publishers, US.
9. Gupta R.R., Kumar M., and Gupta V., (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles*. Vol. 1-3, Springer Verlag, India.
10. Joule, J. A., and Mills, K., (2010). *Heterocyclic Chemistry*. Blackwell Publishers, New York.
11. Smith, M. B., (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*. John Wiley and Sons.
12. Corey, E. J., and Cheng X.-M., (1989). *The Logic of Chemical Synthesis*. John Wiley and Sons.
13. 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.
14. Patil, N. T., and Yamamoto, Y., Coinage Metal-Assisted Synthesis of Heterocycles. *Chemical Reviews*, 2008, 108, 8, 3395-3442.
15. Gribble, G. W., Joule J. A. (2021). *Progress in Heterocyclic Chemistry*, Elsevier - Health Sciences Division, USA.

Course Title: Chemistry of Natural Products

Paper Code: MCHM.522

Credits Hours: 45

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

CLO1: Recognize various types of natural products and their importance.

CLO2: Identify various types of natural products including their properties, occurrence, structure and biosynthesis.

CLO3: Apply the knowledge of natural product synthesis in drug development.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mapping with CLOs
Unit-1 11 Hours	<p>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.</p> <p><i>Importance of isoprene rule in the biosynthesis of terpenes through group presentation.</i></p> <p><i>Advances of terpene based drugs through peer learning.</i></p>	CLO1
Unit-2 11 Hours	<p>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.</p> <p><i>Classroom debate on theory of biogenesis of alkaloids.</i></p> <p><i>Group project on structure-activity relationship based on alkaloid structures.</i></p>	CLO2
Unit-3 11 Hours	<p>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.</p> <p>Coumarins and lignans: Classification, isolation, stereochemistry, biological activity, biosynthesis and synthesis of lignans.</p> <p><i>Group presentation on biological importance of steroids and lignans.</i></p> <p><i>Peer learning of pharmacophore models of natural products.</i></p>	CLO2
Unit-4 12 Hours	<p>Plant pigments: Occurrence, nomenclature and general methods of structure determination. isolation, synthesis and biological activities of anthocyanins, chlorophyll.</p> <p>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.</p> <p><i>Group presentation on biological importance of plant pigments.</i></p> <p><i>Classroom debate on structures and conformation of carbohydrates.</i></p>	CLO3

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

Suggested Readings

1. Bhat, S.V., Nagasampagi, B.A., and Meenakshi, S. (2009). *Natural Product Chemistry and Applications*. Narosa Publishing House, New Delhi.

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

Course Title: Green Chemistry

Paper Code: MCHM.523

Total Contact Hours: 45

Learning outcome: Students will be able to

CLO1: Differentiate various aspects of green chemistry for sustainable development.

CLO2: Utilize ionic liquids, water and solid supported reaction conditions to reduce or eliminate use of volatile organic solvents.

CLO3: Utilize energy efficient MW and ultrasonication in organic synthesis.

CLO4: Apply the judicious use of green reagents for the environmental friendly synthesis of value added chemicals.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mapping with CLOs
Unit-1 11 Hours	<p>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.</p> <p><i>Group project on various green processes successfully employed in chemical industries.</i></p> <p><i>Green chemistry is not costly: Classroom debate.</i></p> <p><i>Chemistry and sustainable lifestyle: Peer Discussion.</i></p>	CLO1
Unit-2 11 Hours	<p>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,</p> <p>Ionic liquids: physicochemical properties, Synthesis of Ionic Liquids, Directed Inorganic and Organometallic Synthesis, formation of oxides, electrochemical synthesis in ionic liquids.</p> <p>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.</p> <p>Supercritical fluids: supercritical CO₂ and its properties, advantages of using CO₂ as solvent, Synthesis of metal nanoparticles, CO₂ as solvent for coatings and lithography, biomaterial processing, and other supercritical fluids.</p> <p><i>Industrial applications of green solvents: peer discussion in the classroom.</i></p> <p><i>Project work on most polluting chemical industries.</i></p> <p><i>Debate on the single use of plastic.</i></p>	CLO2

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. <i>Modern tools as a source of energy for chemical reactions.</i>	CLO3
Unit-4 12 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. <i>Role of Green reagents and their applications for the synthesis of diverse scaffolds through peer learning.</i> <i>Implication and challenges of Biocatalysis in industrial settings through group presentation.</i>	CLO4

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 Priece and Jose Antonio Lopez-Sanchez, Advantages and Limitations of Microwave Reactors: From Chemical Synthesis to the Catalytic Valorization of Biobased Chemicals; Peter Priece *ACS Sustainable Chem. Eng.* 2019, 7, 1, 3–21.

Course Title: Inorganic Spectroscopy and catalysis

Paper Code: MCHM.524

Total Contact Hours: 45

Learning Outcome: The students will be able to

CLO1: Apply properties of f-block elements to analytical and spectroscopic applications

CLO2: Elucidate the inorganic structures using multinuclear-NMR, ESR and Mossbauer Spectroscopy

CLO3: Demonstrate the use of radioanalytical chemistry.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mapping with CLOs
Unit-1 10 Hours	<p>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 superconductors.</p> <p><i>Group discussion on comparative properties and problem solving of lanthanide and Actinide elements.</i></p>	CLO1, CLO2
Unit-2 15 Hours	<p>Nuclear Magnetic Resonance (NMR) and Electron Spin Resonance (ESR) Spectroscopy:</p> <p>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.</p> <p>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 <i>g</i>-tensors, application of transition metal complexes (having one unpaired electron) including biological systems.</p> <p><i>Hand on experience of inorganic complexes for resonance spectroscopy using NMR instrument and structural elucidation.</i></p>	CLO1, CLO2
Unit-3 10 Hours	<p>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.</p> <p><i>Peer discussion on basic parameters and technique implication for structural elucidation of iron and tin contain compounds using Mossbauer Spectroscopy</i></p>	CLO1, CLO2

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. <i>Peer group discussion on Transition metal based industrial processes.</i>	CLO3
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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*, 5th Edition (2012). Elsevier.
10. Kent, B. *Inorganic Chemistry: Reactions, Structures and Mechanisms* (2019). NY Research Press.
11. Close, D. *Principles of Inorganic Chemistry* (2019). Larsen and Keller Education.

Course Title: Solid State Chemistry and Statistical Thermodynamics

L	T	P	Cr
3	0	0	3

Paper Code: MCHM.525

Total Contact Hours: 45

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

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

CLO1: Physicochemical properties, defects in solid, diffraction techniques, electrical and magnetic properties of materials.

CLO2: The relationship between material structure and physical attributes associated with them.

CLO3: Advance applications of these materials.

CLO4: Explain the statistical aspects of system and relate the classical thermodynamics to quantum mechanics.

CLO5: Apprehend and apply partition function in the deduction of thermodynamic properties of chemical systems.

CLO6: Apprehend and apply Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics to the thermodynamic system.

CLO7: Predict and establish the thermodynamic and kinetic aspects of adsorption and catalysis.

Units/ hours	Content	Mappin g with CLOs
Unit-1 15 Hours	<p>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.</p> <p>Semiconductor and Superconductors: Band theory, band gap, metals and semiconductors, intrinsic and extrinsic semiconductors, p-n junctions and other applications (optical activity).</p> <p><i>Demonstration of characterization of these solid state materials like XRD. Relevance of the various aspects of Ferrites in various areas for sustainable development through brainstorming.</i></p>	CLO1,
Unit-2 10 Hours	<p>Nanomaterials: Nanoparticles: zero dimensional nanostructure, homogeneous and heterogeneous nucleation, nanoparticles and their synthesis, nanowires and nanorods: one dimensional nanostructures, thin film and two dimensional nanostructure-preparation techniques.</p> <p>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, magnetic properties of ferrites, applications of ferrites.</p> <p><i>Brainstorming session on the properties of low dimension materials formation.</i></p> <p><i>Concept of Nano dimension materials for modern applications.</i></p> <p><i>Debate on semiconductor materials and their optical and conduction character for device fabrication.</i></p>	CLO2 CLO3

Unit-3 10 Hours	Statistical Thermodynamics: Statistical concepts and examples, postulates of statistical thermodynamics, configurational distribution of energy levels and states, thermodynamic probability and entropy. Partition function, molecular partition function, thermodynamic properties in terms of the molecular partition function for monoatomic gases, rotational, translational, vibrational, electronic and nuclear partition functions for diatomic molecules. <i>Partition function and its correlation to classical thermodynamic evaluation through brainstorming session and peer learning</i>	CLO4 CLO5 CLO6
Unit 4 11 Hours	Theories of Statistical Thermodynamics: Concept of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Relation and Difference between Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Applications of statistical approaches to monoatomic solids, theories of specific heat for solids, chemical equilibrium, Transition state theory and Unimolecular reactions. <i>Demonstrating application of various statistical thermodynamic theories and Debye theory for heat capacity.</i>	CLO7

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.
5. L. K. (2012). *Elements of Statistical Thermodynamics*. Dover Publication Inc.
6. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013). *Principles of Physical Chemistry*. Vishal Publishing Company Nash.
7. Laurendeau, N. M. (2005). *Statistical Thermodynamics: Fundamentals and Applications*. Cambridge University Press.
8. Hill, T. L. (1986). *An Introduction to Statistical Thermodynamics*. Dover Publications Inc.
9. Yu, T. H. (2020). Teaching Thermodynamics with the Quantum Volume J. Chem. Educ., 97 (3), 736-740 DOI: 10.1021/acs.jchemed.9b00742.
10. 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.
11. 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.
12. Novak, I. (2020). Reversible Reactions: Extent of Reaction and Theoretical Yield *J. Chem. Educ.*, 97 (2), 443-447 DOI: 10.1021/acs.jchemed.9b0088.
13. Nelson, K. A., and Bawendi, M. (2008). <https://ocw.mit.edu/courses/chemistry/5-60-thermodynamics-kinetics-spring-2008/video-lectures>.

Course Title: Supramolecular Chemistry

Paper Code: MCHM.526

Total Contact Hours: 45

Learning Outcome: The students will acquire knowledge of

CLO1: Various supramolecular aspects of interaction between two chemical systems.

CLO2: Devising supramolecular systems based on complementarity and preorganizational requirements of the host.

CLO3: Analyze design of hosts for functions based on supramolecular assembly using complementarity and preorganization.

CLO4: Interpret the basic designs of supramolecular machines.

L	T	P	Cr
3	0	0	3

Units/ hours	Content	Mapping with CLOs
Unit 1 11 Hours	<p>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 tetrapyrrolic macrocycles, coenzymes, neurotransmitters, DNA and biochemical self-assembly. Pre-organization and complementarity, receptors, nature of supramolecular interactions.</p> <p>Host-guest chemistry: synthesis and structure of crown ethers, lariat ether and podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, carcerands and hemicarcerands. Concepts of selectivity, macrocyclic, macrobicyclic synthesis and template effects.</p> <p><i>A group activity on design of complementary architectures with explanation of their utility.</i></p>	CLO1
Unit 2 11 Hours	<p>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.</p> <p>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.</p> <p><i>Innovating receptor designs for challenging and emerging sensing application through teamwork and brainstorming.</i></p>	CLO2
Unit 3 11 Hours	<p>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.</p> <p>Dendrimers structure and nomenclature, synthesis and characterization, supramolecular chemistry of dendrimers and its assembly, dendritic nanodevices.</p> <p>Supramolecular polymers including amphiphilic block polymers and molecular imprinter polymers, biological self-assembly in amyloids, actins and fibrin, COF and supramolecular gels.</p> <p><i>Using supramolecular synthons for building self-assembled motifs for purpose by peer learning.</i></p>	CLO3

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. <i>Hands on exercise in groups to develop a theoretical design of a machine tool using organic synthons in supramolecular chemistry.</i>	CLO4
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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 Review*, 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. Feringa, 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: Polymer Chemistry

Paper Code: MCHM.527

L	T	P	Cr
3	0	0	3

Total Lectures: 45

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

CLO1: Elucidate the different mechanisms of polymerization.

CLO2: Demonstrate and compare the various polymer production methods and their key chemical kinetic parameters.

CLO3: Apply the various methods for determination of Number, weight and viscosity average molecular weights.

CLO4: Elucidate and demonstrate the processing of thermoplastic and thermosetting polymers.

CLO5: Apply the polymers for their use in biological and lifestyle applications.

Units/ hours	Content	Mapping with CLOs
UNIT I 13 Hours	<p>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).</p> <p><i>Learning use of various polymerization options by peer learning.</i></p>	CLO1 CLO2
UNIT II 11 Hours	<p>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.</p> <p>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.</p> <p><i>Understanding the polymer molecular mass estimation and distribution using problem solving approach.</i></p>	CLO3
UNIT III 11 Hours	<p>Structure and properties: Configuration of polymer chains. Crystal structure of polymers, morphology of crystalline polymers. Thermal analysis, tensile strength, fatigue, impact, tear resistance, hardness and abrasion resistance.</p> <p>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.</p> <p><i>Analysis of polymer processing parameters using a brainstorming session.</i></p>	CLO4

UNIT IV 10 Hours	<p>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.</p> <p>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.</p> <p><i>Game based and flipped learning of applications of polymers.</i></p>	CLO5
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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

Paper Code: MCHM.528

Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: The student will be able to

CLO1: Inorganic photochemistry and photophysical chemistry.

CLO2: The characterization of transient intermediates by ultrafast modern techniques.

CLO3: The theory of photoreaction.

CLO4: The photochemistry and photophysical chemistry of macromolecules.

Units/ hours	Content	Mapping with CLOs
Unit-1 10 Hours	<p>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.</p> <p><i>Brainstorming on identification of the various photophysical processes where electronic transitions of inorganic molecules are relevant to achieve sustainable development.</i></p>	CLO1,
Unit-2 10 Hours	<p>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.</p> <p><i>Demonstration of the inorganic photochemical reactions and discussion on their potential use as a replacement for artificial photosynthesis.</i></p>	CLO2
Unit-3 10 Hours	<p>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.</p> <p><i>Discussion on recent variants of well-established photochemical processes.</i></p>	CLO3
Unit-4 15 Hours	<p>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, TiO₂ photocatalysis, flash photolysis.</p> <p><i>Application and challenges for the harvesting of energy via value added chemicals.</i></p>	CLO4

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: Advanced Medicinal Chemistry-I

Paper Code: MCMC.404

Course Hours: 45h

L	T	P	Credits
3	0	0	3

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

CLO1: Interpret basic concepts of drugs, their effects and screening.

CLO2: Describe drug interactions with various types of enzymes and receptors.

CLO3: Conceptualize the process of drug discovery and its progress.

Units/ hours	Content	Mappin g with CLOs
Unit 1 10 Hours	<p>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.</p> <p><i>Exercise: Learner will be engaged in group discussion to explain the history of drug discovery.</i></p>	CLO1
Unit 2 11 Hours	<p>Drug discovery: Stages of drug discovery, lead discovery; identification, validation and diversity of drug targets.</p> <p>Biological drug targets: Receptors, types, binding and activation, theories of drug receptor interaction, drug receptor interactions, agonist vs antagonists, artificial enzymes.</p> <p>Measurement and expression of drug effects: Introduction, <i>In-vitro</i> experiments, <i>Ex-vivo</i> experiments, <i>In-vivo</i> experiments.</p> <p><i>Exercise: Learner will be explained about drug interaction and target through molecular modeling studies.</i></p>	CLO2
Unit 3 12 Hours	<p>Prodrug Design and Analog 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 pro drug design.</p> <p>Combating drug resistance: Causes for drug resistance, strategies to combat drug resistance in antibiotics and anticancer therapy, Genetic principles of drug resistance.</p> <p>Analog Design: Introduction, Classical & Non classical, Bio isosteric replacement strategies, rigidanalogs, alteration of chain branching, changes in ring size, ring position isomers, design of stereoisomers and geometric isomers, fragments of a lead molecule, variation in inter atomic distance.</p> <p><i>Exercise : Learner will be engaged in Web based training to familiarize with prodrug and analog design.</i></p>	CLO3

Unit 4 12 Hours	<p>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:</p> <p>b). Anti-hypertensive drugs, Psychoactive drugs, Anticonvulsant drugs, H1 & H2 receptor antagonist, COX1 & COX2 inhibitors, Adrenergic & Cholinergic agents, Antineoplastic and Antiviral agents.</p> <p>c). Stereochemistry and Drug action: Realization that stereo selectivity is a prerequisite for evolution. Role of chirality in selective and specific therapeutic agents. Case studies, enantioselectivity in drug adsorption, metabolism, distribution and elimination.</p> <p><i>Exercise: Learner will be engaged in Group discussion to explain SAR, Mechanism of action and synthesis of drugs.</i></p>	CLO3
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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
- Softwares for *In silico* study
- Google meet

Course Title: Biomolecules and Bioenergetics

Course Code: MBCH.508

Total Hours: 45h

L	T	P	Credits
3	0	0	3

Learning outcomes: Students will be able to

CLO1: Demonstrate the concepts of biomolecules and bioenergetics, various components of cells which are essential for energy generation and their biosynthesis.

CLO2: Apply and effectively communicate scientific reasoning and data analysis in both written and oral forums related to biomolecules and energetics of biochemical processes.

CLO3: Describe and correlate biomolecules and bioenergetics.

Units/ hours	Content	Mapping with CLOs
Unit 1 12 Hours	<p>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.</p> <p>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.</p>	CLO1
Unit 2 11 Hours	<p>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 (alpha-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.</p>	CLO2
Unit 3 10 Hours	<p>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.</p>	CLO3
Unit 4 12 Hours	<p>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.</p>	CLO2, CLO3

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. Williams 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=jLy2K-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

Interdisciplinary Courses (IDCs)

Course Title: Basic Perspectives in Inorganic Chemistry

Paper Code: MCHM.506

Total Contact Hours: 30h

Learning Outcome: The student will able to

CLO1: have expertise of the coordination chemistry of d-group elements and coordination of ions within living organisms.

CLO2: Know the environmental chemistry and metal hydrides as hydrogen energy sources.

L	T	P	Credits
2	0	0	2

Units/ hours	Content	Mappin g with CLOs
Unit-1 7 Hours	Chemistry of d-block elements. coordination chemistry, models and stereochemistry, theories, spectra and bonding. <i>Group discussion and problem solving involving characteristics of transition metals and their compounds.</i>	CLO1,
Unit-2 7 Hours	Ions role in bioscience: ionophores, porphyrin and other tetrapyrrolic macromolecules, coenzymes, neurotransmitters, metal binding to DNA. <i>Brainstorming discussion about essential inorganic elements and their compounds in living organisms.</i>	CLO2
Unit-3 8 Hours	Metals in aqueous environment: Introduction, environmental chemistry, environmental composition, chemical processes, complexes, metal speciation of calcium, copper and mercury, their behaviour in hydrosphere. <i>Discussion on behaviour of metals and complexes in the surrounding environmental sphere.</i>	CLO2
Unit-4 8 Hours	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. <i>Group discussion about current requirements and challenges of renewable energy resources.</i>	CLO2

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: Introduction to Green Chemistry and Sustainability

Paper Code: MCHM.507

Total Contact Hours: 30

L	T	P	Credits
2	0	0	2

Learning objective: Students will be able to

CLO1: Analyze the harmful impact of traditional chemical processes on environment and health.

CLO2: Realize the relevance of Green Chemistry in the context of environmental issues.

CLO3: Apply various tools of Green Chemistry for designing various reactions.

CLO4: Realize the judicious utilization of abundantly available precursors instead of depleting petroleum based feedstocks.

Units/ hours	Content	Mapping with CLOs
Unit-1 7 Hours	<p>Introduction: Adverse effects 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, waste minimization, selection of starting materials etc. Limitations/obstacles in the pursuit of the goals of green chemistry, types of solvent.</p> <p><i>Relevance of the various principles of Green chemistry in various areas for sustainable development through brainstorming.</i></p>	CLO1, CLO2
Unit-2 7 Hours	<p>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.</p> <p><i>Various emerging energy efficient tools and their heating mechanism for conducting chemical reactions through collaborative approach.</i></p>	CLO1, CLO2 CLO3
Unit-3 8 Hours	<p>Green solvents: Ionic liquids: properties and advantages, use of ionic liquids as solvent as well as catalyst, recyclability of ionic liquids. Solvent-free synthesis.</p> <p><i>Recyclability of ionic liquids through demonstration and discussion on their potential use as a replacement for halogenated volatile organic solvents.</i></p>	CLO2, CLO3
Unit-4 8 Hours	<p>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.</p> <p><i>Progress and challenges for the conversion of biomass into value added chemicals through peer group learning.</i></p>	CLO4

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.
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Course Title: Chemistry of Nanomaterials and Fabrication

Paper Code: MCHM.508

Total Contact Hours: 30

Learning Outcome:

CLO1: The students will acquire knowledge of Nanotechnology,

CLO2: Fabrication and characterization of nanomaterials,

CLO3: Properties and applications of nanomaterials.

L	T	P	Credits
2	0	0	2

Units/ hours	Content	Mappin g with CLOs
Unit-1 7 Hours	<p>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.</p> <p><i>Relevance of the various aspects of Nano chemistry in various areas for sustainable development through brainstorming.</i></p>	CLO1,
Unit-2 7 Hours	<p>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.</p> <p><i>Variousadvanced techniques for nanomaterials characterization and their formation mechanism through collaborative approach.</i></p>	CLO2
Unit-3 8 Hours	<p>Nanomaterials and properties: Influence of nucleation rate on the size of the crystals- macroscopic to microscopic crystals and nanocrystals - large surface to volume ratio. Metals (Au, Ag) - metal oxides (TiO₂, CeO₂, ZnO etc.) - semiconductors (Si, Ge, CdS, ZnSe) - carbon nanotubes (CNT) - ceramics and composites - dilute magnetic semiconductor- biological system - DNA and RNA - lipids - size dependent properties - mechanical, physical and chemical properties.</p> <p><i>Concept of Nano dimension materials fabrication.</i></p>	CLO3

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. <i>Concept of Nano dimension materials for modern applications.</i>	CLO3
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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*, Wiley-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.

Course Title: General Laboratory Practices

Paper Code: MCHM.509

Total Contact Hours: 30

Learning Outcome: The students will acquire knowledge of

CLO1: Good laboratory practices

CLO2: Quality control and Quality assurance

CLO3: Chemical, biological and radiation hazards in laboratory and safety.

CLO4: General knowledge of analytical sample preparation.

L	T	P	Credits
2	0	0	2

Units/ hours	Content	Mappin g with CLOs
Unit 1 7 Hours	<p>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.</p> <p><i>Regulatory requirement through gaming a laboratory for GLP through dramatization.</i></p>	CLO1
Unit 2 8 Hours	<p>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.</p> <p><i>Understanding the quality deliverability of disciplinary laboratories through team brainstorming.</i></p>	CLO2
Unit 3 8 Hours	<p>Safety and Hazard Analysis: Chemical classification of hazards, Radiation hazard, AERB regulation for Fire and its prevention, biosafety and biohazard. Weapons of Mass destruction.</p> <p><i>Understanding National and international regulatory requirements of chemical and bio- hazards through hands-on inspection of laboratories.</i></p>	CLO3
Unit 4 7 Hours	<p>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.</p> <p><i>Understanding the selection of analytical procedures for analysis and sample preparation methods using peer learning.</i></p>	CLO4

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

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.

4. http://www.who.int/water_sanitation_health/resourcesquality/wqmchap9.pdf.
5. <https://www.unece.org/fileadmin/DAM/env/water/publications/documents/guidancelaboratories.pdf>.
6. <https://www.ugc.ac.in/oldpdf/xiplanpdf/disposalofradioactiv.pdf>.
7. https://www.mea.gov.in/Uploads/PublicationDocs/148_The-Weapons-Mass-destruction-And-Delivery-Systems-Act-2005.pdf.
8. Westgard, J. O., Barry, P. L. (2016). *Basic QC Practices: Training in Statistical Quality Control for Medical Laboratories*, 4th ed., Westgard Quality Corporation.
9. Kenkel, J. (2014). *Analytical Chemistry for Technicians*, 4th ed., CRC Press.
10. Konieczka, P., Namiesnik, J., (2018). *Quality Assurance and Quality Control in the Analytical Chemical Laboratory: A Practical Approach*, 2nd ed. CRC Press.
11. WHO (2011). *Laboratory Quality Management System Handbook*.
12. Zaman, G., (2018). *Quality Control in Laboratory*, Intech Open Publishing.
13. Hasnain, M.S., Beg, S., (2019). *Pharmaceutical Quality by Design: Principles and Applications*, Elsevier Science.

Course Title: Chemistry of Drug Design and Synthesis

Paper Code: MCHM.510

Total Contact Hours: 30

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

CLO1: Rationalize the basis of drug design, drug action and drug metabolism.

CLO2: Apply the knowledge to design and synthesize different drug molecules.

CLO3: Interpret the mechanism of action of different classes of drugs.

L	T	P	Cr
2	0	0	2

Units/ hours	Content	Mapping with CLOs
Unit-1 8 Hours	<p>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.</p> <p><i>Apply the knowledge of drug-receptor interactions in drug design through peer learning.</i></p>	CLO1
Unit-2 7 Hours	<p>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.</p> <p><i>Class discussion of molecular modelling in structure based and ligand based drug design approach.</i></p>	CLO2
Unit-3 7 Hours	<p>Drug Metabolism: Biotransformation of drugs, enzymes responsible for bio-transformations, microsomal and non-microsomal mechanisms; Factors influencing enzyme induction and inhibition, Factors affecting drug metabolism; Models to study drug metabolism, Adverse drug reactions; toxic reactions, allergic reactions.</p> <p><i>Usefulness of different models to study drug metabolism through peer discussion.</i></p>	CLO2
Unit-4 8 Hours	<p>Mechanism of action and synthesis of various drugs: Introduction to parasitic and infectious diseases, Mechanism of action of anti-tuberculosis drugs, anti-HIV drugs, antimalarial 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.</p> <p><i>Recent advances on anticancer and antibiotic drug synthesis through brainstorming.</i></p>	CLO3

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 Modelling 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.

Course Title: Project Report

Paper Code: MCHM.529

Total Contact Hours: 120

Learning Outcome: The student would be able to

CLO1: Understand the lacunas in the methodology to experimentation.

CLO2: Independently plan and execute experiments in the laboratory set-up

CLO3: Analyze and interpret the results obtained through different experiments.

CLO4: Apply expertise and specific skills in the frontier area of research.

As per the defined objectives in the research proposal, 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 project report will be prepared as per the university guidelines for PG diploma in Chemistry in consultation with the supervisor. Project would be verified for plagiarism and submitted for evaluation by the committee.

Course Title: Chemical Laboratory Techniques

Paper Code: MCHM.530

Total Contact Hours: 120

L	T	P	Cr
4	0	0	4

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

CLO1: Trained in the operation and maintenance of chemicals & common apparatus used in laboratories. Familiarize them to develop skills in common laboratory techniques; train them in the procedures of procurement and storage of laboratory equipment, apparatus, glass wares and chemicals; enable them to follow appropriate disposal procedures and safety measures required for chemistry laboratories.

CLO2: Enabled to follow appropriate disposal procedures and safety measures required for chemistry laboratories. It will produce well trained Staff /Technicians to work in chemistry labs, especially Pharma industries or other small scale industries.

CLO3: to perform the basic and research experiments. To impart knowledge of all safety measures in the chemistry laboratory, proper disposal of chemicals, chemical wastes and other waste materials; awareness about the handling of corrosive chemicals, lab accidents, fire extinguishers and other safety means; Knowledge of computer for proper organization and management of chemistry laboratories, minor electronic equipment, maintain lab record, inventory etc.

Units/ hours	Content	Mapping with CLOs
Unit-1 15 Hours	<p>Introduction of Chemistry Lab: General introduction of chemistry laboratory, common instruction for safe working in chemical laboratories, Lab design, Storage, ventilation, lighting, fume, cupboard, arrangement of store, Safety provisions, Organization of practical work, Maintenance of laboratory, equipment/ apparatus Cleaning of laboratories and preparation room.</p> <p>Introduction of Lab Apparatus: <i>Glass apparatus</i> - Beaker, Test tube, boiling tube, funnel, separating funnel, filtration flask, round bottom flask, flat bottom flask, condenser Liebig flask, watch glass etc. measuring conical or condenser, petridish, desiccator. <i>Volumetric Apparatus</i> - Measuring cylinder, burette, pipette, Volumetric flask, analytical balance, single-pan electronic balance/ electrical analytical balance etc. <i>Miscellaneous apparatus</i>- Buchner funnel, Bunsen burner, burette stand, retort clamp, china dish/evaporating basin, wire gauze, cork borers, filter pumps, crucible, mohr clip, pipe clay triangle, pestle and mortar, spirit lamp, spatulas, thermometer, pH meter/pH paper etc. and laboratory centrifuge. <i>Apparatus for heating</i>: Bunsen burner, water bath, oil bath hot plate, sand bath, hot air oven, heating mantle etc. <i>Handling and storage of glass apparatus.</i> Solution Preparation: Water as a solvent, types of water, solutions, components of a solution, types of solution, solubility, concentration of solutions: percentage, molarity, normality, molality (in ppm) calculation of masses and volumes for preparation of solutions solids, liquids. <i>Group discussion on use of chemicals and problem solving of solutions of different normality/concentrations.</i></p>	CLO1, CLO2
Unit-2 15 Hours	<ol style="list-style-type: none"> 1. Handling of common laboratory equipment 2. Cork boring experiment 3. Calibration of volumetric glassware 4. Weighing of chemicals using analytical balance 5. Preparation of solutions, indicators and reagents. 6. Preparation of buffer solutions and determination of their pH Values. 7. Preparation of some organic compounds and determination of their boiling point and melting point. <p><i>Hand on experience of common laboratory and research equipment.</i></p>	CLO1, CLO2

<p>Unit-3</p> <p>15 Hours</p>	<p>Common Laboratory Techniques: <i>Refluxing:</i> Apparatus with interchangeable ground glass joints (Quick fit). <i>Filtration:</i> Techniques and filter media, filter paper, simple filtration. <i>Recrystallization:</i> Choice of solvent and precautions with flammable solvents. <i>Distillation:</i> recovery of solvents through partial distillation, distillation under reduced pressure, and <i>Determination of Boiling Point.</i> Chemistry Laboratory Safety: <i>Fire Hazards:</i> Causes of fires, classification of fires, fire prevention protocols and measures, fire alarms, fire escapes, fire Extinguishers and their uses. <i>Chemical Hazards:</i> Classification and handling of hazardous chemicals, storage of chemicals, transfer from large containers. <i>Gas Hazards:</i> usage of LPG and CNG safer in the laboratory, detection and handling of Gas Leakage, health hazards of gases. Use of Computer in Laboratory: Hardware in computer, CPU, I/O devices, data input, data processing, data output, application MS office software and Internet. Stock and Inventory Control: Arranging stock, locating and referencing, shelf arrangement of stock, order books, inventory. Files and Records <i>Filing Systems-</i> Classification of files, filing methods, filing system for equipment and chemicals, filing of printed and written material, preparation of lab manuals. <i>Records system :</i> Stock records, recording stock (used and misused), record of use of listed poisons, record of use of alcohol, record of breakages, information about equipment serial numbers, record maintenance, miscellaneous records. <i>Activity 1:</i> Cleaning of laboratories and preparation room. <i>Activity 2:</i> Classification of apparatus in store. <i>Activity 3:</i> Cleaning of glassware. <i>Activity 4:</i> Organization of practical work. <i>Activity 5:</i> A brief report on Safety provisions in laboratories.</p> <p><i>Peer discussion on Laboratory Techniques and significance of records of experimental data.</i></p>	<p>CLO1, CLO2</p>
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Unit-4 15 Hours	1. Purification of aniline by distillation method 2. Crystallization of various compounds and their TLC study 3. Column chromatographic method for separation of compounds 4. Simple acid-base titration. 5. Preparation of distilled/deionized water. 6. Preparation of inorganic double salts. 7. Experiments based on chromatography Activity 1: Classification of chemicals in laboratory/store. Activity 2: Classification of hazardous chemicals based on the information given on the labels. Activity 3: Preparation of comparative chart. Activity 4: To learn the use of a carbon dioxide fire extinguisher. Activity 5: Preparation of stock register on MS-Excel. <i>Brainstorming discussion on various lab practicals.</i>	CLO2 CLO3
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Suggested Readings

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.

Course Title: Intellectual Property Right

Paper Code: MCHM.531

Total Lecture: 60

L	T	P	Cr
4	0	0	4

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

CLO1: Understand the importance of Intellectual Property Rights, its various types and scope for the protection of his/her novel creations.

CLO2: Critically analyse the inventiveness of his/her work over the prior art available.

CLO3: Think and develop ethical values regarding copyrights

CLO4: Familiar with various agencies and treaties regarding Intellectual Property Rights

Units/ hours	Content	Mapping with CLOs
Unit-1 14 Hours	<p>Introduction: Intellectual property and need for its protection, Intellectual Property Rights (IPR), Types of intellectual property; Industrial property & copyrights and related rights. IPR in India and abroad, promotion and protection concepts.</p> <p>Impact of IPR on development, health & agriculture, IPR in biotechnology: New plant varieties, protection needs and laws.</p>	CLO1
Unit-2 16 Hours	<p>Patents: Characteristics of patent. Patentable and non-patentable inventions in India, patent applications and their types; specification and claims, granting of patent, Transfer Commercialization Related Aspects, Indian Patent Act 1970, and amendments, Opposition to the grant of patent applications and post grant oppositions processes.</p> <p>Trademarks: Types, purpose and function of trademark, registration and protection aspects.</p> <p>Industrial Designs: Registration and protection.</p> <p>Geographical Indicators: Geographical indicators and their protection, difference between geographical indication and trademark.</p> <p>Trade Secrets: Advantages and limitations.</p>	CLO1, CLO2
Unit-3 15 Hours	<p>Copyrights: Copyrightable works; ownership of copyright; Exploiting Fair Use concept in copyright especially in academics and research. Infringement of copyright.</p> <p>Related Rights: Difference between copyright and related rights, celebrity rights.</p> <p>Academic integrity: Plagiarism and UGC regulations 2018, Plagiarism detection softwares.</p>	CLO2, CLO3
Unit-4 15 Hours	<p>Organizations, agencies and Treaties: Territoriality of IPR; International Conventions in IPR; Role of World Trade Organization (WTO) and World Intellectual Property Organization (WIPO), The patent corporation treaty (PCT), GATT (General Agreement on Tariff and Trade), TRIPs (Trade Related Intellectual</p>	CLO4

	Property Rights) agreement, TRIMS (Trade Related Investment Measures) and GATS (General Agreement on Trades in Services).	
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Mode of Transaction: Lecture, Demonstration, Lecture cum demonstration, Dialogue Mode, Experimentation, Problem solving, Seminar.

Suggested Readings:

1. Simran R. Gurnani. Intellectual Property Rights, C. Jamnadas & Co. (2021).
2. V K Ahuja, "Law Relating to Intellectual Property Rights", Lexis Nexis (2017).
3. *Copyright Law*, Vaver, Dav, Toronto: Irwin Law, ISBN 1-55221-034-0, 2000.
4. *Intellectual Property*, Drahos, Peter, Adlershot et.al. Darmouth, ISBN 1840147407, 1999.
5. *Intellectual Property: Patents, Copyright trademarks and allied rights*, Cornish, William R, London: Sweet and Maxwell, 4th edition, ISBN: 0421635401, 1999.
6. *Intellectual Property Reading Material*, World Intellectual Property Organization, 2nd edition, ISBN: 92-805-0756-7, 1998.
7. *Patents, trademarks, and related rights; national and international protection*, Ladas, Stephen P, Cambridge, MA: Harvard University Press, ISBN: 06746577756, 1975.
8. *Universal's The Patent Act (39 of 1970) with amendments*-Universal Law publishing 2005.

Course Title: Modern Instrumental Methods

Paper Code: MCHM.532

Total Lecture: 60

L	T	P	Cr
4	0	0	4

Learning Outcome: After the completion of the course, students will gain knowledge on

CLO1: Principles and analytical applications of modern instrumentation.

CLO2: Principles of various chromatography and their application for purification of compounds.

CLO3: Principles of various radioanalytical methods and application of different radioisotopes in industry.

CLO4: Demonstration of various imaging techniques and hands-on training on several spectroscopic techniques.

Units/ hours	Content	Mapping with CLOs
Unit-1 15 Hours	<p>Principles and Instrumentation: Analytical applications of following techniques: Atomic Absorption spectroscopy, Flame photometry, Inductively coupled plasma-Atomic Emission spectroscopy, Scanning Electron Microscopy.</p> <p><i>Peer discussion on principles of modern instrumentation.</i> <i>Classroom discussion on various analytical applications of modern instrumentation.</i></p>	CLO1
Unit-2 15 Hours	<p>Chromatography: Gas solid Chromatography, Gas liquid Chromatography, High performance liquid chromatography, ion exchange chromatography, paper chromatography, thin layer chromatography, column chromatography, gel permeation chromatography.</p> <p><i>Demonstration of chromatographic techniques in the laboratory.</i> <i>Classroom discussion on the principles of various chromatography for purification of compounds.</i></p>	CLO2
Unit-3 10 Hours	<p>Radioanalytical Methods: X-ray diffraction methods, Neutron activation analysis, isotope dilution analysis, Radiometric titrations, particle induced X-ray Emission, Use of radioisotopes - in industry, agriculture and physicochemical studies.</p> <p><i>Principles of various radioanalytical methods through classroom discussion.</i> <i>Application of different radioisotopes in industry through peer learning.</i></p>	CLO3
Unit-4 20 Hours	<p>Imaging Techniques: Electron Microscopy including TEM, STEM, and FESEM with dark field and bright field imaging.</p> <p>Industrial visits and Hands-on Training and demonstration practical based on following techniques: HPLC, GCMS, NMR, FTIR, XRD, TGA, AAS and SEM.</p> <p><i>Demonstration of various imaging techniques.</i> <i>Hands-on training on several spectroscopic techniques.</i></p>	CLO3

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

Suggested Readings

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

<u>Semester-III</u>							
S. No.	Course Code	Course Title	Course Type	L	T	P	Cr
1	MCHM.599-1	Dissertation Part-I	SB	0	0	40	20
		Total		0	0	40	20

Course Title: Dissertation Part-I

Paper Code: MCHM.599-1

Total Contact Hours: 600

Course Outcome: The student would be able to

CLO1: Investigate various aspects related to the chemistry problem.

CLO2: Generate interest in frontier areas of research in chemistry and pursue for higher studies.

CLO3: 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 the 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.

<u>Semester-IV</u>							
S. No.	Course Code	Course Title	Course Type	L	T	P	Cr
1	MCHM.599-2	Dissertation Part-II	SB	0	0	40	20
		Total		0	0	40	20

C: Core Course, **SB:** Skill-Based Course, **CF:** Compulsory Foundation, **DE:** Discipline Elective Courses, **VAC:** Value-added Course

Course Title: Dissertation Part-II

Paper Code: MCHM.599-2

Total Contact Hours: 600

Learning Outcome: The student would be able to

CLO1: Understand the lacunas in the methodology to experimentation.

CLO2: Independently plan and execute experiments in the laboratory set-up.

CLO3: Analyze and interpret the results obtained through different experiments.

CLO4: 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.