

**Syllabus for Multi-Disciplinary Minor Degree  
In  
Chemical Sciences**

**Under the National Education Policy (NEP 2020)**

**in  
(2023-2024)**



**Offered by**

**DEPARTMENT OF CHEMISTRY**

**INSTITUTE OF CHEMICAL TECHNOLOGY**

(University Under Section-3 of UGC Act, 1956)

**Elite Status and Center for Excellence**

**Government of Maharashtra**

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## A. Preamble:

Chemistry is known as the ‘central science’ – a sound understanding of the interactions between molecules is critical in all the technical applications. Understanding the fundamentals of Chemistry is the first step towards designing high throughput synthetic methodologies for fine and bulk chemicals, pharmaceutical components, plastics, etc. All industrial progress relies primarily on the improved materials provided by the chemical industry. Applications based on the chemical sciences are bound to play an indispensable role in achieving sustainable development goals at a global level.

The present module of Multidisciplinary Minor (MDM) degree in Chemical Sciences is offered by the Department of Chemistry, Institute of Chemical Technology (ICT) under the aegis of the National Education Policy (NEP 2020). The aim of the Chemical Sciences MDM degree is to equip Chemical Engineering and Chemical Technology undergraduates with a thorough understanding of the concepts and applications of Chemistry. The salient features of the MDM degree in Chemical Sciences are as follows:

**Industry relevance:** The bulk and fine manufacturing industries rely heavily on their trained experts to bridge the gap between concepts and technology. The MDM aims to equip students for diverse roles in numerous industries such as pharmaceuticals, polymers, dyes, and textile industries

**Innovation and Entrepreneurship:** The national objectives of self-reliance are driving the economy towards a setup where entrepreneurial ventures will be more important. With the growth in demand for locally manufactured chemicals and in accordance with the Institute’s legacy of producing industrialists and entrepreneurs, students will be able to successfully combine the expertise in Chemistry and technology to address this expanding market.

**Research and Development:** The future of research in interdisciplinary areas with greater coordination between the scientists and technologists. The students will comprehend and combine both aspects through their training to be competent researchers on a global level.

**Sustainable development:** The current challenges of pollution and non-renewable feedstocks can only be addressed through well-trained chemical experts. Development of clean technologies and energy-efficient transportation can be achieved only through application of chemical knowledge. Chemistry can play a pivotal role in ensuring food security and access to health care – key factors in alleviating poverty.

## B. Programme Specific Outcomes:

### Programme Specific Outcomes (PSOs) for Chemical Sciences (MDM)

PSO1	<b>Foundation of Organic Chemistry:</b> Understand the structure and properties of hydrocarbons (including aliphatic, aromatics, heterocyclics) to enable problem solving related to the largest class of industrially relevant compounds and processes related to their manufacture
PSO2	<b>Foundation of Physical Chemistry:</b> Use the principles of kinetics, interfacial phenomena, and the underlying thermodynamic concepts to link basic chemical sciences and engineering principles for solving real life problems
PSO3	<b>Foundation of Computational Chemistry:</b> Apply modern computational theories and methods to model chemical systems from the molecular scale to bulk scale – critical in developing advanced understanding
PSO4	<b>Foundation of Catalysis:</b> Understand the diverse applications of catalysis and the developments in the field to enable application of cutting-edge chemical technology on a large scale
PSO5	<b>Conduct investigations of complex problems:</b> Identify, formulate, review research literature, and analyze complex real-life problems using chemical know-how Use research-based knowledge in chemical sciences and research methods including design of experiments, analysis, and interpretation of data to unfold complex problems from industry and academia and provide working solutions.
PSO6	<b>Societal Applications of Chemistry:</b> Apply reasoning informed by the existing knowledge pool to convert into a quantitative framework, collect relevant information and address various societal issues using chemical tools

**C. Intake: Minimum 15 and Maximum 35**

**(the intake criteria is subject to the norms prescribed by the Institute)**

- D. **Eligibility criteria:** The courses offered require a basic understanding of the principles of Chemistry at Std XII (HSC or equivalent) level. The students enrolled for the B. Chem. Engg. / B. Tech. (Chemical Technology) programs of the Institute of Chemical Technology are eligible due the present criteria for admission. The allotment to the MDM degree and/or change, if any, in MDM after Sem-III examination will be as per the Institute's rules.

In case the candidate wishes to opt for the MDM degree in Chemical Sciences but does not meet the eligibility criterion, he/she/they may have to acquire the same by successfully completing equivalent courses and providing evidence for the same.

- E. **Pedagogy:** The courses will be taught in a combination of classroom lectures and experiential learning modules. Laboratory demonstrations will be incorporated wherever required for enhanced understanding. Courses like Computational Chemistry will involve practical exercises as an important component.
- F. **Evaluation:** The students will be assessed based on a combination of continuous assessment and end-semester test. The continuous assessment could be incorporated in the form of quizzes, assignments, presentations, group projects, etc. The evaluation policies are subject to the norms prescribed by the Institute.

**G. Structure of the multidisciplinary minor (MDM) degree program in Chemical Sciences:**

Subject Code	Sem	Subject	Credits	Hrs./Week			Marks for various Exams			
				L	T	P	CA	MS	ES	Total
CHT 1003	III	Chemical Kinetics	02	2	0	0	20	30	50	100
CHT 1004	IV	Interfacial Chemistry	02	2	0	0	20	30	50	100
CHT 1005	V	Organic Synthesis	04	3	1	0	20	30	50	100
CHT 1006	VI	Organic Spectroscopy	02	2	0	0	20	30	50	100
CHT 1007	VII	Computational Chemistry	02	2	0	0	20	30	50	100
CHT 1008	VIII	Organometallic Chemistry and Catalysis	02	2	0	0	20	30	50	100
		<b>Total</b>	14							

**H. Faculty members:**

- 1) Chemical Kinetics – Prof. R. V. Jayaram
- 2) Interfacial Chemistry – Prof. R. V. Jayaram
- 3) Organic Synthesis – Dr. A. R. Kapdi
- 4) Organic Spectroscopy – Prof. A Chaskar / Visiting faculty
- 5) Computational Chemistry – Dr. R. V. Pinjari
- 6) Organometallic Chemistry and Catalysis – Prof. B. M. Bhanage / Dr. A. Kapdi

**I. Detailed syllabus:**

	<b>Course Code:</b> <b>CHT 1003</b>	<b>Course Title: Chemical Kinetics</b>	<b>Credits = 2</b>		
			<b>L</b>	<b>T</b>	<b>P</b>
	<b>Semester: III</b>	<b>Total contact hours: 30</b>	<b>2</b>	<b>0</b>	<b>0</b>
<b>List of Prerequisite Courses</b>					
Std XII Chemistry, Chemistry-I					
<b>List of Courses where this course will be prerequisite</b>					
Interfacial Chemistry (CHT 1004)					
<b>Description of relevance of this course in the MDM in Chemical Sciences</b>					
The course covers the key concepts of three of the principal topics in chemical kinetics. This will help to understand how fast a reaction can go. Understanding of reaction rates and kinetic parameters affecting the same are critical for designing and controlling many industrially relevant processes.					
<b>Course Contents (Topics and subtopics)</b>					<b>Hours</b>
1	Chemical kinetics – Introduction, concept of reaction rates and order, experimental methods in kinetic studies, differential and integral methods to formulate rate equations of zero, first and second order				<b>03</b>
2	Complex reactions- parallel, consecutive, and reversible reactions, order, and molecularity				<b>03</b>
3	Kinetics and reaction mechanism- steady state and rate determining step Mechanism of thermal photochemical chain reactions, polymerization reactions, branched chain reactions and kinetics of enzyme catalysis				<b>06</b>
4	Kinetics of surface reactions – Adsorption, Hinshelwood, and Ridel models of surface reactions				<b>02</b>
5	Theories of reaction rates and temperature effects- Collision theory and TST Theory of unimolecular reactions				<b>04</b>
6	Kinetics of reactions in solutions- solvent effects and effects of ionic strength Kinetic isotope effect				<b>04</b>
8	Fast reactions and reactions in molecular beams – experimental techniques				<b>03</b>
9	Kinetics of solid-state reactions				<b>02</b>
10	Applications – Food industry, Pharmaceuticals, Industrial synthesis				<b>03</b>
					<b>30</b>
<b>List of Textbooks / Reference Books</b>					
1	Chemical Kinetics – K.J. Laidler, Pearson, 2003				
2	Principles of Chemical Kinetics- J.C.House, Publisher Wm C. Brown, 1997				
3	Chemical Kinetics: The Study of Reaction Rates in Solution, Kenneth Antonio Connors, John Wiley & Sons, 1990				
4	Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis Arnaut, Elsevier, 2021				
<b>Course Outcomes (students will be able to....)</b>					
CO1	Express the rate laws for different mechanisms using appropriate models				K2
CO2	Apply the rate laws to chemical reactions and processes				K3

CO3	Analyze the kinetic aspects of chemical processes taking place on the interfacial electrode surface	K3
CO4	Compare the theoretically predicted rates with the rates computed experimentally	K3
CO5	Modify the kinetic parameters to improve the selectivity or yield of given reaction / process	K3
CO6	Evaluate the kinetic model by comparing the experimentally observed data with the proposed rate law	K4

<b>Mapping of Course Outcomes (COs) with Programme Outcomes (PSOs)</b>						
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	3	2	1	1	2
CO2	2	3	2	1	1	2
CO3	2	3	1	2	2	3
CO4	1	3	3	2	2	1
CO5	3	2	3	3	2	3
CO6	2	3	1	2	1	1

3-Strong Contribution; 2-Moderate Contribution; 1-Low Contribution

	<b>Course Code:</b> <b>CHT 1004</b>	<b>Course Title: Interfacial Chemistry</b>	<b>Credits = 2</b>		
			<b>L</b>	<b>T</b>	<b>P</b>
	<b>Semester: IV</b>	<b>Total contact hours: 30</b>	<b>2</b>	<b>0</b>	<b>0</b>
<b>List of Prerequisite Courses</b>					
Chemical Kinetics (CHT 1003)					
<b>List of Courses where this course will be prerequisite</b>					
Organometallic Chemistry and Catalysis (CHT 1008)					
<b>Description of relevance of this course in the MDM in Chemical Sciences</b>					
The chemistry at interfaces, surfaces and disperse systems is important in governing stability/reactivity in various materials. The course introduces fundamentals of interfacial chemistry which can be applied to heterogeneous catalysis, electrochemistry, separation processes and allied fields.					
<b>Course Contents (Topics and subtopics)</b>					<b>Hours</b>
1	<b>Surface and interfacial Chemistry</b> – Introduction, surface tension and surface free energy, methods of determining surface and interfacial tensions				<b>02</b>
2	<b>Thermodynamics of surfaces</b> – Surface excess, Gibbs adsorption equation, curved surfaces- bubbles, droplets and foams, Kelvin, Young Laplace and Thomson equations, homogeneous nucleation				<b>05</b>
3	<b>Liquid- liquid and solid liquid interfaces</b> – Contact angle, wetting and spreading, adhesion and cohesion, contact angle measurements and hysteresis				<b>04</b>
4	<b>Surfactants:</b> Types, adsorption at surfaces and interfaces, surfactant aggregates, factors affecting aggregation phenomena				<b>06</b>
5	Modern developments in surfactants synthesis and applications				<b>02</b>
6	Industrial applications of surfactants				<b>03</b>
7	Environmental effects of surfactants				<b>02</b>
8	<b>Disperse systems</b> - Emulsions microemulsions and foams, Thermodynamics and stability, HLB values, Colloids - preparation, stability, characterization, surface charges and electrical double layer				<b>06</b>
					<b>30</b>
<b>List of Textbooks / Reference Books</b>					
1	Introduction to colloid and surface chemistry – D. J. Shaw, Butterworth Publications, 2000				
2	Surfaces interfaces and colloids- Drew Myers- Wiley VCH , 1999				
3	Surfactants and interfacial phenomena- Milton J Rosen – Wiley Interscience , 2004				
4	Industrial utilization of surfactants principles and applications – M.J. Rosen and M Dahanayake, AOCS Press , 2000				
5	Foundations of Colloid science – Robert J Hunter – Oxford university Press, 2001				
6	Interfacial Science: An Introduction, Second Edition, Geoffrey Barnes and Ian Gentle, Oxford University Press, 2011				
<b>Course Outcomes (students will be able to....)</b>					
CO1	Identify the importance of interfacial phenomena in influencing the behaviour of disperse systems				K1
CO2	Understand the variation of structural features at the interface and the resulting effect on properties				K2
CO3	Utilize the information from various characterization techniques to understand interfacial features				K3
CO4	Explain the interfacial properties by applying various models to the interfacial systems				K2

CO5	Design surfactants / colloids for a given application using the various surface properties	K3
CO	Justify the observed macroscopic behaviour based on interfacial properties	K4

Mapping of Course Outcomes (COs) with Programme Outcomes (PSOs)						
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	1	2	2	2	1	1
CO2	1	2	2	2	1	1
CO3	1	3	3	1	2	2
CO4	2	3	2	1	3	1
CO5	1	2	2	2	3	2
CO6	1	3	3	3	2	2

3-Strong Contribution; 2-Moderate Contribution; 1-Low Contribution



	<b>Course Code:</b> <b>CHT 1005</b>	<b>Course Title: Organic Synthesis</b>	<b>Credits = 4</b>		
	<b>Semester: V</b>		<b>Total contact hours: 60</b>	<b>L</b>	<b>T</b>
			<b>3</b>	<b>1</b>	<b>0</b>
<b>List of Prerequisite Courses</b>					
B. Chem. Engg. – Applied Chemistry (CHT 1251) or equivalent; B. Tech. – Organic Chemistry (CHT 1407) or equivalent					
<b>List of Courses where this course will be prerequisite</b>					
Organic Spectroscopy (CHT 1006), Organometallic Chemistry and Catalysis (CHT 1008)					
<b>Description of relevance of this course in the MDM in Chemical Sciences</b>					
To acquaint the students with concepts related to fundamentals of Organic Chemistry including reaction mechanisms, organic transformations, types of reactions, selectivity of chemical transformations, stereochemical implications of organic reactions, functional group identification and reactions so that they are perfectly aligned to apply the same for future courses and in their professional career					
<b>Course Contents (Topics and subtopics)</b>					<b>Hours</b>
1	<b>Chemistry of Carbonyl Compounds</b> Concept of acidity and tautomerism of carbonyl compounds, General methods of preparation and Nucleophilic Addition reactions Enolate chemistry, Aldol and related condensation reactions, Michael reaction, Robinson annulation, Claisen condensation, Dieckmann condensation, Mannich reaction.				<b>10</b>
2	<b>Haloalkanes:</b> General reactions. Mechanisms of nucleophilic substitutions reactions (SN1 & SN2) and elimination reactions.				<b>10</b>
3	<b>Heteroaromatic compounds:</b> Basic structures and common names, comparison of electronic and structural properties to benzenoid compounds, Reactivity and synthetic routes Pyrrole, Furan, Thiophene, Pyridine.				<b>12</b>
4	<b>Named Organic Reactions:</b> Perkin reaction (Mauvine synthesis-dyes), Fischer indole synthesis (Dyes), Jacobson Corey epoxide synthesis (Pharmaceuticals), Ziegler Natta polymerization (Polymer), Multicomponent reactions, Maillard reaction (Foods), Strecker amino acid synthesis (Pharmaceuticals & Foods), Wittig reactions, Prilezhaev reaction				<b>10</b>
5	<b>Stereochemistry of Organic Compounds</b> Containing one and two asymmetric carbon atoms, Stereo descriptors – R/S, E/Z, erythro and thero, Conformation – Ethane and butane. Enantiomers and Diastereomers, meso compounds, different representations of stereoisomers – Saw-horse, Newmann, Wedge and dash and Fischer and their interconversions				<b>10</b>
6	<b>Chemistry of important natural products:</b> Terpenes, steroids, carotenoids/prostaglandins				<b>8</b>
					<b>60</b>
<b>List of Textbooks / Reference Books</b>					
1	Clayden, J., Greeves, N., Warren, S.; Organic Chemistry; 2nd ed.; Oxford University Press (2012)				
2	Graham Solomons, T. W.; Fryhle, Craig B.; Snyder, Scott A. Organic Chemistry; 12th Ed.; John Wiley & Sons. Inc. (2016)				
3	Smith, M. B.; March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure; 7th ed.; Wiley, India (2015)				
4	Carey F. A., Sundberg, R. J. Advanced Organic Chemistry: Part A: Structure and Mechanisms; 5th ed.; Springer (2005)				

5	Carey F. A., Sundberg, R. J.; Advanced Organic Chemistry: Part B: Reaction and Synthesis; 5th ed.; Springer (2007)	
6	Wade, L. G.; Simek, J. W.; Singh, M. S. Organic Chemistry; 9th Ed.; Pearson Education (2019)	
7	Eliel, E. L. Stereochemistry of Carbon Compounds; McGraw-Hill (2001)	
8	Bruice, Paula, Y. Organic Chemistry; 8th Ed.; Pearson Education (2020)	
9	Bhat, S. V., Nagasampagi, B. A., Meenakshi, S. Natural Products Chemistry and Applications. Narosa publishing house (2009)	
<b>Course Outcomes (students will be able to....)</b>		
CO1	Identify structures of organic compounds and write their IUPAC names correctly	K2
CO2	Understand organic chemistry reactions related to aliphatic as well as aromatic compounds as well as decipher the outcome of a given organic transformation	K2
CO3	List the properties and synthetic routes, and decipher outcomes of various transformations involving heterocycles	K3
CO4	Apply the knowledge obtained through the course to predict the outcome of reactions and devise solutions to unknown problems	K3
CO5	Appreciate the stereochemical implications of organic compounds and visualize and appreciate the chirality concept	K3
CO6	Interpret and analyze reactions having different functionalities to predict products and design synthetic protocols	K4

<b>Mapping of Course Outcomes (COs) with Programme Outcomes (PSOs)</b>						
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	1	1	2	2	1
CO2	2	1	1	2	2	1
CO3	3	2	2	1	3	1
CO4	3	1	2	2	2	1
CO5	3	2	1	3	1	2
CO6	3	2	2	2	2	2

3-Strong Contribution; 2-Moderate Contribution; 1-Low Contribution

	<b>Course Code:</b> <b>CHT 1006</b>	<b>Course Title: Organic Spectroscopy</b>	<b>Credits =</b> <b>2</b>		
	<b>Semester: VI</b>	<b>Total contact hours: 30</b>	<b>L</b>	<b>T</b>	<b>P</b>
			<b>2</b>	<b>0</b>	<b>0</b>
<b>List of Prerequisite Courses</b>					
B. Chem. Engg. – Applied Chemistry (CHT 1251) or equivalent; B. Tech. – Analytical Chemistry (CHT 1406) or equivalent					
<b>List of Courses where this course will be prerequisite</b>					
<b>Description of relevance of this course in the MDM degree in Chemical Sciences</b>					
This course aims to introduce the students to the concepts of organic spectroscopy. The course content is designed to familiarize the students with various spectroscopic techniques used for the structural elucidation of organic molecules.					
<b>Course Contents (Topics and subtopics)</b>					<b>Hours</b>
1	<b>Ultraviolet (U.V.) Spectroscopy:</b> Introduction, spectrophotometer, Beer-Lambert's law, Energy absorption and electronic transitions, Terms used in U.V. spectroscopy (Chromophore, auxochrome, bathochromic shift, hypochromic shift, hyperchromic and hypochromic shift), Woodward – Fieser Rules for dienes, enones and aromatic compounds,				<b>6</b>
2	<b>Infrared spectroscopy:</b> Vibrational transitions, Selection rule, Modes of stretching and bending, FT-IR (Fourier Transform Infra-Red) spectroscopy. Group frequencies, Factors affecting IR group frequency, NIR spectroscopy, Applications of vibrational spectroscopy in structural elucidation of organic compounds.				<b>6</b>
3	<b>NMR (Nuclear Magnetic Resonance) Spectroscopy</b> A. <b><sup>1</sup>H NMR Spectroscopy:</b> Basic principle, Nuclear spin states and magnetic moments, Chemical shifts, Factors affecting the chemical shift, Shielding mechanism and anisotropic effects. B. <b><sup>13</sup>C NMR Spectroscopy:</b> Elementary idea, Chemical shift, Calculation of approximate chemical shift values, coupling constants, Interpretation of simple CMR spectra, Proton coupled and decoupled <sup>13</sup> C NMR spectra.				<b>10</b>
4	<b>Mass Spectrometry:</b> Introduction, Ion production, Fragmentation, Stevenson's rule, Radical site and Charge site-initiated cleavage, Rearrangements, Cleavage associated with common functional groups, Molecular ion peak, Metastable ion peak, Nitrogen rule, LRMS and HRMS, Isotopic abundance and Interpretation of mass spectra.				<b>8</b>
					<b>30</b>
<b>List of Textbooks / Reference Books</b>					
1	Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman, G.S. Kriz, J.R. Vyvyan, Cengage Learning India Pvt Ltd , 2009				
2	Spectrometric Identification of Organic Compounds, Robert M. Silverstein, Francis X. Webster, Wiley , 2005				
3	Organic Spectroscopy: William Kemp, Palgrave , 1975				
4	Principles of NMR in one and Two Dimensions: R.R. Ernst, G. Bodenhausen, A. Wokaun: Oxford Science Publication , 1987				

<b>Course Outcomes (students will be able to....)</b>		
CO1	Understand the general principles of various spectroscopic techniques used for characterization of organic molecules	K2
CO2	Assign the spectroscopic data to structural features of molecules	K3
CO3	Understand the theory of Nuclear Magnetic Resonance spectroscopy and its applications to structural problems	K2
CO4	Predict the fragmentation of alkanes, alkyl aromatics, alcohols, ketones using the principle of McLafferty rearrangement, and mass spectrometry	K3
CO5	Solve problems based on UV, IR, NMR & MS Spectroscopy for interpretation of the structure.	K4
CO6	Choose the optimum spectroscopic technique/s for identification and structure elucidation of a given compound	K3

<b>Mapping of Course Outcomes (COs) with Programme Outcomes (PSOs)</b>						
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	1	1	2	2	1
CO2	2	1	1	2	2	1
CO3	3	2	2	1	3	1
CO4	3	2	2	2	2	2
CO5	3	1	2	2	2	1
CO6	3	2	1	3	1	2

3-Strong Contribution; 2-Moderate Contribution; 1-Low Contribution

	<b>Course Code:</b> <b>CHT 1007</b>	<b>Course Title: Computational Chemistry</b>	<b>Credits = 2</b>		
	<b>Semester: VII</b>		<b>Total contact hours: 30</b>	<b>L</b>	<b>T</b>
			<b>2</b>	<b>0</b>	<b>0</b>
<b>List of Prerequisite Courses</b>					
Standard XII <sup>th</sup> Mathematics (Calculus and Matrix Algebra), Chemistry					
<b>List of Courses where this course will be prerequisite</b>					
<b>Description of relevance of this course in the MDM in Chemical Sciences</b>					
Quantum chemistry gives the molecular level understanding of the chemical reactions and the properties of moderated sized isolated molecules, while molecular mechanics can be used for the studying the supramolecules and ensembles. The course will provide a brief introduction to applying computational packages to molecules and supramolecular assemblies.					
<b>Course Contents (Topics and subtopics)</b>					<b>Hours</b>
1	Introduction to Computational Chemistry, Basic concepts				<b>2</b>
2	<b>Historical background of quantum mechanics</b> - failure of classical theory, wave particle duality, uncertainty principle, Postulates of Quantum mechanics, probabilistic interpretation of wave function, Schrodinger wave equation, Eigen values and operators.				<b>4</b>
3	<b>Applications of Schrodinger equation</b> – particle in a box, harmonic oscillator				<b>4</b>

	<b>H and H like atoms</b> - two particle problem, Schrodinger equation in spherical coordinates, representation of orbitals, radial and angular plots, probability functions	
4	<b>Chemical bonding</b> - Born-Oppenheimer approximation, LCAO and MO theory	<b>4</b>
5	<b>Electronic structure - methods:</b> SCF Theory, Energy of Slater Determinant, Basis Set Approximation, Basis Sets, Hartree-Fock Approximation	<b>6</b>
6	Semiempirical Methods, Huckell Theory	<b>4</b>
7	<b>Force fields</b> , potential energy functions, inter and intramolecular interactions, empirical parameters. <b>Molecular mechanics</b> calculations, energy minimization, conformational analysis	<b>4</b>
8	Applications in Drug Designing, QSAR, and Catalysis.	<b>2</b>
		<b>30</b>

#### List of Textbooks / Reference Books

1	Alan Hinchliffe, Molecular Modelling for Beginners, 2nd Ed. Wiley & Sons, 2008.
2	Frank Jensen, Introduction to Computational Chemistry, Wiley & Sons, 1999.
3	Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Ed. Wiley & Sons, New York.
4	Daan Frenkel & Berend Smit, Understanding Molecular Simulation, AP, NY, 2002.
5	Andrew R. Leach, Molecular Modelling: Principles and Applications, 2nd Ed., Prentice Hall, 2001.
6	James E. House, Fundamental of Quantum Chemistry, 2nd Ed. Academic Press, 2004.

#### Course Outcomes (students will be able to....)

CO1	Define the computational techniques currently used to predict the structure and properties of molecules	K2
CO2	Apply semi-empirical / ab initio techniques to model structure and properties of molecules	K3
CO3	Apply molecular dynamics techniques for modelling larger systems and elucidate their properties	K3
CO4	Compare the output of the various computational methods to explain the experimental observations	K4
CO5	Choose the optimum level of theory for computing properties of the systems	K4
CO6	Design the computational protocol for predicting the outputs of chemical reactions and processes	K4

#### Mapping of Course Outcomes (COs) with Programme Outcomes (PSOs)

	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	1	2	3	1	2	1
CO2	1	2	3	1	2	1
CO3	1	2	3	2	2	2
CO4	1	3	3	1	1	1
CO5	1	2	3	2	1	1

CO6	2	2	3	2	1	1
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3-Strong Contribution; 2-Moderate Contribution; 1-Low Contribution

	<b>Course Code:</b> <b>CHT 1008</b>	<b>Course Title: Organometallic Chemistry and Catalysis</b>	<b>Credits = 2</b>		
	<b>Semester: VIII</b>	<b>Total contact hours: 30</b>	<b>L</b>	<b>T</b>	<b>P</b>
			<b>2</b>	<b>0</b>	<b>0</b>
<b>List of Prerequisite Courses</b>					
Organic Synthesis (CHT 1005)					
<b>List of Courses where this course will be prerequisite</b>					
<b>Description of relevance of this course in the MDM in Chemical Sciences</b>					
To acquaint the students with the concepts of organometallic chemistry which is the basis of all the catalytic processes either known in academia or industries. The course will allow students to appreciate the science behind how catalytic processes help expedite synthesis.					
<b>Course Contents (Topics and subtopics)</b>					<b>Hours</b>
1	<b>General Properties of Organometallic Complexes:</b> 18- electron rule and its limitation, Electron counting in reactions, Bridged complexes, Metal-metal bond. Associative-Dissociative mechanisms				<b>6</b>
2	<b>Complexes of <math>\pi</math>-Bound Ligands:</b> Back bonding concept for explaining metal-alkene and alkyne interactions. Alkene and Alkyne complexes allyl complexes, Diene complexes. Ziegler-Natta Polymerization, SHOP (Shell Higher Olefin Process), Catalytic Hydrogenation				<b>10</b>
3	<b>Carbonyls Complexes:</b> Back bonding concept for explaining metal-carbonyl interactions. Metal complexes of CO ligands, Dissociative substitution, Associative mechanism. Substitution reactions of Metal-CO complexes. Formylation (Monsanto Acetic Acid Synthesis), Hydroformylation (Otto Roelen Process)				<b>10</b>
4	<b>Organometallic chemistry for meeting future challenges:</b> Environment remediation for CO <sub>2</sub> utilization and depolymerization				<b>4</b>
					<b>30</b>
<b>List of Textbooks / Reference Books</b>					
1	The organometallic chemistry of the transition metals, Robert H. Crabtree, John Wiley & Sons				
2	Organometallic Chemistry of Transition elements: F. P. Pruchnik: Springer				
3	Organometallic reagents in Organic Synthesis: Paul R. Jenkins: Oxford Science Publication				
<b>Course Outcomes (students will be able to....)</b>					
CO1	Learn the basic concepts of how catalysis works				K1
CO2	Understand the basic properties for organometallic compounds				K2
CO3	Explain the observed properties based on structure and bonding in organometallics				K2
CO4	Explain the experimental observations by proposing plausible mechanisms for catalytic reactions				K3
CO5	Select the suitable organometallic compounds for applications as catalysts in organic transformations				K3

CO6	Develop synthesis and characterization protocols for organometallics based on the desired structure and applications	K3
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<b>Mapping of Course Outcomes (COs) with Programme Outcomes (PSOs)</b>						
	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	2	1	2	2	2
CO2	2	2	1	2	2	2
CO3	2	2	1	3	2	2
CO4	1	1	2	3	1	2
CO5	1	1	2	3	1	2
CO6	1	1	1	3	2	2

3-Strong Contribution; 2-Moderate Contribution; 1-Low Contribution