PROPOSED SYLLABUS REVISION FOR

M.TECH

in

ADVANCED CHEMICAL SYNTHESIS AND ANALYSIS

SUBMITTED TO

THE DEAN (ACADEMICS)
INDIAN INSTITUTE OF TECHNOLOGY DELHI

BY

DEPARTMENT OF CHEMISTRY
INDIAN INSTITUTE OF TECHNOLOGY DELHI

FEBRUARY 2015

DEPARTMENT OF CHEMISTRY
INDIAN INSTITUTE OF TECHNOLOGY, DELHI
REVISED SYLLABUS FOR
M.TECH. IN "ADVANCED CHEMICAL SYNTHESIS & ANALYSIS"

Name of the Programme	**M.Tech. in "Advanced Chemical Synthesis and Analysis"**
Name of the Department offering the Programme	**Chemistry**

Distribution of Total Credits

Program core PC	Program/Open elective PE/OE	Total Credits
42	12	54

Semester wise Distribution of credits

Sem I	Sem II	Sem III	Sem IV	Total Credits
18	18	9	9	54

M.Tech. in "Advanced Chemical Synthesis and Analysis"

Sem	Courses (Number, Abbreviated title, L-T-P, credits)						Lecture courses	Contact h/week				Credits
								L	T	P	Total	
I	CYL721 Design & Synthesis (3-0-0) 3	CYL726 Chem-informatics (3-0-0) 3	CYL731 Separation & Electro-analytical (3-0-0) 3	CYP722 Lab on synthesis (0-0-6) 3	**PE/OE-1** (3-0-0) 3	**PE-2** (3-0-0) 3	5	15	0	6	21	**18**
II	CYL724 Inorganic Materials (3-0-0) 3	CYL729 Material Character-ization (3-0-0) 3	CYL737 Applied Spectro-scopy (3-0-0) 3	CYP728 Instru. Lab. (0-0-6) 3	**PE/OE-3** (3-0-0) 3	**PE-4** (3-0-0) 3	5	15	0	6	21	**18**
III	CYD806 Major Project Part - I (0-0-18) 9						0	0	0	18	18	**9**
IV	CYD806 Major Project Part - II (0-0-18) 9						0	0	0	18	18	**9**

Total = 54

Scheduling of Courses

Semester I

	Course No.	Title	Type	L-T-P	Credits
1	CYL721	Design and Synthesis of Organic Molecules	PC	3-0-0	3
2	CYL726	Cheminformatics and Molecular Modelling	PC	3-0-0	3
3	CYL731	Chemical Separation and Electroanalytical Methods	PC	3-0-0	3
4	CYP722	Synthesis of Organic and Inorganic Compounds	PC	0-0-6	3
5		Elective - 1	PE/OE	3-0-0	3
6		Elective - 2	PE/OE	3-0-0	3
			Total Credits		**18**

Semester II

1	CYL724	Synthesis of Industrially Important Inorganic Materials	PC	3-0-0	3
2	CYL729	Material Characterization	PC	3-0-0	3
3	CYL737	Applied Spectroscopy	PC	3-0-0	3
4	CYP728	Instrumentation Laboratory	PC	0-0-6	3
5		Elective - 3	PE/OE	3-0-0	3
6.		Elective - 4	PE/OE	3-0-0	3
			Total Credits		**18**

Semester III

1	CYD806	Major Project Part - I		0-0-18	**9**
			Total Credits		**9**

Semester IV

1	CYD807	Major Project Part - II		0-0-18	**9**
			Total Credits		**9**

A. List of program Electives for M.Tech in "Advanced Chemical Synthesis and Analysis".

PROGRAM ELECTIVES

	Course No.	Title	L-T-P	Credits
1	CYL723	Principles and practice of NMR and Optical Spectroscopy	3-0-0	3
2	CYL733	Chemistry of Industrial Catalysts	3-0-0	3
3	CYL734	Chemistry of Nanostructured Materials	3-0-0	3
4	CYL738	Applications of p-block elements and their compounds	3-0-0	3
5	CYL739/ CYL695	Applied Biocatalysis	3-0-0	3
6	CYL740/ CYL675	Chemistry of Heterocyclic Compounds	3-0-0	3
7	CYL741	Organo and organometallic catalysis	3-0-0	3
8	CYL742	Reagents in Synthetic Transformations	3-0-0	3
9	CYL801	Molecular Modelling and Simulations: Concepts and Techniques	3-0-0	3
10	CYD799	Minor project	0-0-6	3

B. List of NEW courses if any being proposed

	Course No.	Title	L-T-P	
1	CYL724	Synthesis of Industrially Important Inorganic Materials	3-0-0	3 (PC)
2.	CYL737	Applied Spectroscopy	3-0-0	3 (PC)
3	CYL738	Applications of p-block elements and their compounds	3-0-0	3 (PE)
4	CYL739	Applied Biocatalysis	3-0-0	3 (PE)
5	CYL740	Chemistry of Heterocyclic Compounds	3-0-0	3 (PE)
6	CYL741	Organo and organometallic catalysis	3-0-0	3 (PE)
7	CYL742	Reagents in Synthetic Transformations	3-0-0	3 (PE)
8	CYL801	Molecular Modelling and Simulations: Concepts and Techniques	3-0-0	3 (PE)

List of courses, if the course title or LTP have undergone change for the revised programme

1	CYL721	Design and Synthesis of Organic Molecules	PC	3-0-0	3
2	CYL731	Chemical Separation and Electroanalytical Methods	PC	3-0-0	3
3	CYL729	Material Characterization	PC	3-0-0	3

C. List of courses where the course contents have changed

All the old PC and PE courses have been rewritten with minor changes in contents on account of revision/updating of M.Tech. curriculum.

Details of the Courses

First Semester

CYL721: Design and Synthesis of Organic Molecules (3-0-0)

Selectivity in organic synthesis: chemo-, regio, stereo- and enantioselectivity. Target-oriented synthesis: Designing organic synthesis, Retrosynthetic analysis, disconnetion approach, linear and convergent synthesis. Diversity-oriented synthesis: concept of forward-synthetic analysis, appendage diversity, skeletal diversity, stereochemical diversity, complexity and diversity. Asymmetric Synthesis: Use of chiral auxiliaries, chiron approach. Principles and use of enzymes in the syntheis of industrially important sugar / fatty acid esters, sugar nucleotide derivatives ; enantiomeric pure compounds and biobased platform chemicals.

CYL726: Cheminformatics and Molecular Modelling (3-0-0)

Chemistry & Information technology, chemical / biochemical data collation, retrieval, analysis & interpretation, hypothesis generation & validation, development of structure activity/property relationships, artificial intelligence techniques in chemistry. Building molecules on a computer, quantum and molecular mechanics methods for geometry optimization, Simulation methods for molecules and materials.

CYL731: Chemical Separation and Electroanalytical Methods (3-0-0)

Theory and applications of equilibrium and nonequilibrium separation techniques. Extraction, countercurrent distribution, gas chromatography, column and plane chromatographic techniques, electrophoresis, ultracentrifugation, and other separation methods, Modern analytical and separation techniques used in biochemical analysis. Principles of electro-chemical methods, electrochemical reactions, steady-state and potential step techniques; polarography, cyclic voltammetry, chrono methods, rotating disc and ring disc electrodes, concepts and applications of AC impedance techniques.

CYP722: Laboratory on Synthesis (0-0-6)

Single, double and multi-stage preparation of organic, inorganic and organometallic compounds; experiments involving the concepts of protecting groups and selectivity; identification of compounds through thin-layer chromatography and their purification by column chromatography. Characterization of synthesized compounds using IR, UV, ^{1}H- NMR and mass spectromteric techniques.

Elective - 1

Elective - 2

Second Semester

CYL724: Synthesis of Industrially Important Inorganic Materials (3-0-0)

Modern methods applied in the synthesis of inorganic, organometallic and polymer materials. Handling of air and moisture sensitive compounds, dry box, glove bag, Schlenk line and vacuum line techniques. Methods of purification of and handling of reactive industrial gases. Methods of purification of inorganic compounds and crystallization of solids for X-ray analysis. General strategies, brief outline of theory and methodology used for the synthesis of inorganic/organometallic molecules to materials including macromolecules. Emphasis will be placed how to adopt appropriate synthetic routes to control shape and size of the final product, ranging from amorphous materials, porous solids, thin films, large single crystals, and special forms of nanomaterials. A few examples of detailed synthesis will be highlighted in each category of materials.

CYL729: Material Characterization (3-0-0)

Compositional analysis of solid materials by X-ray and electron microscopic techniques. Basic concepts of diffraction techniques (powder and single crystal) in elucidating the crystal structures organic, inorganic and hybrid materials. Applications of electron microscopic techniques (scanning and transmission) for morphological and nanostructural features. Thermal analytical methods for correlating structural information and monitoring phase transition. Emphasis will be placed on the above techniques for industrially important materials and the interpretation and evaluation of the results obtained by various methods.

CYL737: Applied Spectroscopy (3-0-0)

Applications of advanced 1D-NMR techniques such as nOe, 1D ^{13}C-NMR (including APT and DEPT) techniques, multinuclear NMR spectroscopy, 2D NMR techniques (COSY, HETCOR, HSQC, HMBC, NOESY, ROESY etc.) for the structural and stereochemical determination of organic compounds. Introduction to various types of ionizations (such as EI, CI, MALDI, field ionization/desorption, electrospray ionization) and analyzers (such as quadrupole, time of flight, triple quadupole, QqTOF, ion-trap) in mass spectrometry for MS, MS/MS and MS^n applications. Determination of peptide sequencing using mass spectrometric techniques.

CYP728: Instrumentation Laboratory (0-0-6)

Experiments based on Instrumental methods of chemical analysis involving spectroscopy, microscopy and thermal methods.

Elective - 3

Elective - 4

Third Semester

CYD806 Major Project Part - I

Fourth Semester

CYD807 Major Project Part - II

Departmental Electives [*Any four to be selected*: Two in I semester and two in II semester; CYD799 to be opted only in Semester - II]

CYL723: Principles and practice of NMR and Optical Spectroscopy (3-0-0)

Fundamentals of FT NMR spectroscopy, relation between structure and NMR properties, one-dimensional spectroscopy (1H, 13C, DEPT, steady state NOE, saturation transfer) and an introduction to two-dimensional NMR (COSY, NOESY, and HSQC) and their use in structure elucidation. Principles and analytical applications of optical spectroscopic methods including atomic absorption and emission, UV-Visible, IR absorption, scattering, and luminescence.

CYL733: Chemistry of Industrial Catalysis (3-0-0)

Fundamental aspects of catalysis - Homogeneous and Heterogeneous catalysis. The role of catalytic processes in modern chemical manufacturing - organometallic catalysts - catalysis in organic polymer chemistry - catalysis in petroleum industry - catalysis in environmental control.

CYL734: Chemistry of Nanostructured Materials (3-0-0)

Introduction; fundamentals of nanomaterials science, surface science for nanomaterials, colloidal chemistry; Synthesis, preparation and fabrication: chemical routes, self assembly methods, biomimetic and electrochemical approaches; Size controls properties (optical, electronic and magnetic properties of materials) - Applications (carbon nanotubes and nanoporous zeolites; Quantum Dots, basic ideas of nanodevices).

CYL738: Applications of p-block elements (3-0-0)

Introduction, Structure, bonding and recent discussions on d orbital participation. Boranes, carboranes and metallaboranes and their use in BNCT and as control rods in nuclear reactors, modern electron counting methods such as Jemmis rules, chemistry of B(0) and B(1). GaAs, GaN, $InSnO_3$: Synthesis and applications in solar cells, LED and as transparent conducting materials. Fullerenes, nanotubes, graphene, silicates, aluminosilicates, zeolites and their applications. Silicones and their industrial applications. Si(II) and Ge(II) chemistry. NHC's and their use in stabilizing main group compounds. Nitrogen based fertilizers, Ammonia, Haber-Bosch Process, nitrogen based explosives, hydrazines as rockel fuels, applications of azides and pentazenium. Phosphorus based fertilizer processes, phosphorus based pesticides, phosphorus-nitrogen compounds as multidentate ligands, superbases, dendrimer cores and polymers. Phosphines and their industrial uses. Frustrated Lewis acid bases as catalysts. Superacids and their uses. Sulphonamides, industrial applications of sulfur and selenium. Fluorine in pharmaceuticals, fluoropolymers.

CYL739/ CYL695: Applied Biocatalysis (3-0-0)

Introduction to enzymes and enzyme catalysed reactions. Classification and mechanism of reaction. Purification and characterization of enzymes. Michelis Menten kinetics, Industrial enzymes. Applications of enzymes in diagnostics, analysis, biosensors and other industrial processes and bio-transformations.Enzyme structure determination, stability and stabilisation. Enzyme immobilization and concept of enzyme engineering. Nanobiocatalysis.

CYL740/ CYL675: Chemistry of Heterocyclic Compounds (3-0-0)

Chemistry of heterocyclic compounds containing one, two and three heteroatoms. Total synthesis of representative natural products.

CYL741: Organo and Organometallic Catalysis (3-0-0)

Introduction. Enamine catalysis. Iminium catalysis. Asymmetric proton catalysis. Ammonium ions as chiral templates. Chiral Lewis bases as catalysts. Asymmetric acyl transfer reactions. Ylide based reactions. Transition metal catalyzed reactions. C-H activation. *N*-Heterocyclic carbenes.

CYL742: Reagents in Synthetic Transformations (3-0-0)

The course will cover the applications of various oxidation and reduction reactions in organic chemistry with special emphasis on advance reagents that are used for selective transformations. Use of organolithium and organoboron compounds in organic synthesis and olefin metathesis will also serve as a part of the course.

CYD799: Minor Project (0-0-6)

CYL801: Molecular Modelling and Simulations: Concepts and Techniques (3-0-0)

Review of Basic Concepts: Length and Time Scales, Intermolecular Interactions and Potential Energy Surfaces, Evaluation of Long-range interactions. Static and Dynamic Properties of Simple and Complex Liquids. Molecular Dynamics: Microcanonical and other ensembles; Constrained simulations; non-equilibrium approaches. Monte Carlo Methods: Random Numbers and Random Walks, Metropolis Algorithm in various ensembles, Biased Monte Carlo Schemes. Free Energy Estimations: Mapping Phase Diagrams, Generating Free Energy Landscapes, Collective Variables. Rare Event Simulations and Reaction Dynamics. Advanced Topics: First principles molecular dynamics, Quantum Monte Carlo methods, Coarse-Graining and Multiscale Simulations for Nanoscale Systems, Quantum mechanics/molecular mechanics (QM/MM) approaches.

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	CHEMISTRY
2.	**Course Title** *(< 45 characters)*	DESIGN AND SYNTHESIS OF ORGANIC MOLECULES
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL721
6.	**Status** (*category* for *program*)	PROGRAM CORE

7.	**Pre-requisites** (course no./title)	NIL

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	15% with CYL562
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	Existing CYL721

9.	**Not allowed for** (indicate program names)	NIL

10.	**Frequency of offering**	☐ Every sem ☒ 1st sem ☐ 2nd sem ☐ Either sem

11.	**Faculty who will teach the course** NALIN PANT, N G RAMESH, V HARIDAS, NIDHI JAIN, RAVI P SINGH, SHIVAJI GHOLAP, S K KHARE, TANMAY DUTTA	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)***:** This course aims to focus on synthesis based on advanced level organic chemistry and also would include the applications of enzymes in organic synthesis.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** Selectivity in organic synthesis: chemo-, regio, stereo- and enantioselectivity. Target-oriented synthesis: Designing organic synthesis, Retrosynthetic analysis, disconnetion approach, linear and convergent synthesis. Diversity-oriented synthesis: concept of forward-synthetic analysis, appendage diversity, skeletal diversity, stereochemical diversity, complexity and diversity. Asymmetric Synthesis: Use of chiral catalysts, organocatalysis, chiron approach and N-heterocyclic carbenes. Principles and use of enzymes in the syntheis of industrially important sugar / fatty acid esters, sugar nucleotide derivatives ; enantiomeric pure compounds and biobased platform chemicals

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Selectivity in Organic Synthesis	10
2	Target Oriented Synthesis	8
3	Diversity-oriented synthesis	8
4	Asymmetric synthesis	10
5	Prinicpals of enzymes mediated recations	1
6	Enzyme based syhthesis of sugar / fatty acid esters, sugar nucleotide derivatives ; enantiomeric pure compounds	2
7	Biobased production of basic/ platform chemicals	2
8	Industrial examples and success stories	1
9		
10		
11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

Nil

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
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9		
10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Jonathan Clayden, Nick Greeves, Stuart Warren,
   Organic Chemistry, Second edition, Oxford, 2012.
2. Paul Wyatt, Stuart Warren
   Organic Synthesis - Strategy and Control, First Edition, Wiley, 2006.
3. George S Zweifel, Michael H Nantz
   Modern ORganic Synthesis - An Introduction, W. H. Freeman and Compnay, 2006.
4 Karlheinz Drauz and Harald Gröger
   Enzyme Catalysis in Organic Synthesis, Wiley, 2012
5 Stanley M. Roberts and G. Casy
   Biocatalysts for Fine Chemicals Synthesis, Wiley, 1999
6 Kenneth M. Nicholas.
   Selective Catalysis for Renewable Feedstocks and Chemicals (Topics in Current Chemistry), Springer 2014

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	No
19.2	Hardware	No
19.3	Teaching aides (videos, etc.)	No
19.4	Laboratory	No
19.5	Equipment	No
19.6	Classroom infrastructure	Overhead Projector
19.7	Site visits	No

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	PRINCIPLES AND PRACTICE OF OPTICAL AND NMR SPECTROSCOPY
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL723
6.	**Status** (*category* for *program*)	Program Elective

7.	**Pre-requisites** (course no./title)	None

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	NO
8.2	Overlap with any UG/PG course of other Dept./Centre	NO
8.3	Supercedes any existing course	CYL723

9.	**Not allowed for** (indicate program names)	None

10.	**Frequency of offering**	☐Every sem ☒1st sem ☐2nd sem ☐Either sem

11.	**Faculty who will teach the course** P. K. Chowdhury, S. Deep, N. D. Kurur, and S. Pandey	
12.	**Will the course require any visiting faculty?**	NO

13.	**Course objective** *(about 50 words)***:** Optical and NMR spectroscopy are by far the most used tools in chemical analysis. The principles of the two forms of spectroscopy are outlined in this course.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** Fundamentals of FT NMR spectroscopy, relation between structure and NMR properties, one-dimensional spectroscopy (1H, 13C, DEPT, steady state NOE, saturation transfer) and an introduction to two-dimensional NMR (COSY, NOESY, and HSQC) and their use in structure elucidation. Principles and analytical applications of optical spectroscopic methods including atomic absorption and emission, UV-Visible, IR absorption, scattering, and luminescence.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	FT NMR	5
2	Relation between structure and NMR properties	2
3	One dimensional NMR	7
4	Multidimensional NMR	7
5	Principles of optical spectroscopy	5
6	Atomic spectroscopy	4
7	UV-Vis spectroscopy	4
8	IR spectroscopy	2
9	Scattering	3
10	Luminescence	3
11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
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10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. H. Gunther, NMR spectroscopy
2. J. K. M. Sanders and B. K. Hunter, Modern NMR spectroscopy
3. M. J. Pelletier, Analytical Applications of Raman Spectroscopy
4. J. R. Lakowicz, Principles of Fluorescence spectroscopy
5. J. Workman and A. Springsteen, Applied spectroscopy
6. M. J. K. Thomas and D. J. Ando, Ultraviolet and Visible spectroscopy: Analytical Chemistry by Open learning
7. K. C. Thompson, Atomic absorption, fluorescence, and flame emission spectroscopy: A practical approach
8. J. D. Ingle and S. R. Crouch, Spectrochemical analysis

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	Room with OHP and projector to seat 25 students
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	CHEMISTRY
2.	**Course Title** *(< 45 characters)*	SYNTHESIS OF INDUSTRIALLY IMPORTANT INORGANIC MATERIALS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL724
6.	**Status** (*category* for *program*)	Program Core

7.	**Pre-requisites** (course no./title)	Nil

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	No
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	No

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☐1st sem ☒2nd sem ☐Either sem

11.	**Faculty who will teach the course** S Nagendran, Ravi Shankar, J D Singh, A Ramanan	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)***:** To provide working knowledge of how to design industrially important materials from molecular precursors. Emphasis will be placed on how to choose appropriate precursors to obtain a product with desired composition and properties with desired micro/nano structures.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** Modern methods applied in the synthesis of inorganic, organometallic and polymer materials. Handling of air and moisture sensitive compounds, dry box, glove bag, Schlenk line and vacuum line techniques. Methods of purification of and handling of reactive industrial gases. Methods of purification of inorganic compounds and crystallization of solids for X-ray analysis. General strategies, brief outline of theory and methodology used for the synthesis of inorganic/organometallic molecules to materials including macromolecules. Emphasis will be placed how to adopt appropriate synthetic routes to control shape and size of the final product, ranging from amorphous materials, porous

	solids, thin films, large single crystals, and special forms of nanomaterials. A few examples of detailed synthesis will be highlighted in each category of materials.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Introduction to Industrial examples (molecules and materials) and their success stories	2
2	Design aspects of polynucleating organic ligands of variable donor abilities and functionalities for their usage in chemical sensor technology with particular interest in quantification of biologically and environmentally crucial inorganic and organic anions and metal cations.	4
3	Design of novel coordination and organometallic polymers	4
4	New synthetic routes that can control shape and size of the final product, ranging from amorphous materials to large single crystals, and special forms of nanomaterials, porous materials and thin films.	4
5	Solid-state reactions	2
6	Formation of solids from gas phase (Chemical vapor deposition, aerosol process)	2
7	Formation of solids from solution - Sol-gel chemistry and hydrothermal synthesis	6
8	Preparation and modification Inorganic Polymers of group 14, 15 and 16 elements including conducting polymers. Handling of Air-sensitive compounds	10
9	Porous materials	4
10	Nanostructured materials	4
11	Synthesis of inorganic, organometallic compounds and hybrid materials of catalytic, technological and medicinal significance using a variety of synthetic methods.	
12		
COURSE TOTAL *(14 times 'L')*		

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
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10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Schubert, U. and Husing N., Synthesis of Inorganic Materials, Wiley-VCH (2000)
2. Shriver, D. F., The Manipulation of Air Sensitive Compounds: The best source of information on inert atmosphere and high vacuum methods and Schlenk techniques,
3. Angelici, R. J. Synthesis and Techniques in Inorganic Chemistry, 2nd Ed. University Science Books: N.Y. (1986)
4. Chandrasekhar, V., Inorganic polymers, Wiley-VCH (2008).

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	7.
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	CHEMISTRY
2.	**Course Title** *(< 45 characters)*	CHEMINFORMATICS AND MOLECULAR MODELING
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL726
6.	**Status** (*category* for *program*)	Program Core

7.	**Pre-requisites** (course no./title)	None

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	CYL668 would provide introduction to molecular simulations.
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	CYL726

9.	**Not allowed for** (indicate program names)	Nil
10.	**Frequency of offering**	☐ Every sem ☒ 1st sem ☐ 2nd sem ☐ Either sem
11.	**Faculty who will teach the course** B. Jayaram, C. Chakravarty, H. K. Kashyap	
12.	**Will the course require any visiting faculty?**	No

13. Course objective *(about 50 words)*:

To prepare students for data analysis, hypothesis generation and validation and to acquaint students with latest trends in computer aided molecule/material design

14. Course contents *(about 100 words) (Include laboratory/design activities)*:

Chemistry & Information technology, chemical / biochemical data collation, retrieval, analysis & interpretation, hypothesis generation & validation, development of structure activity/property relationships, artificial intelligence techniques in chemistry. Building molecules on a computer, quantum and molecular mechanics methods for geometry optimization, Simulation methods for molecules and materials

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Chemistry & IT: Introduction	2
2	Data Collation, Analysis, Interpretation, Hypothesis generation/ validation	6
3	1D,2D,3D QSAR/QSPR	3
4	Applications of Artificial Intelligence Techniques in Chemistry/Biochemistry	4
5	Quantum Chemical calculations	5
6	Molecular Mechanical Calculations	5
7	Molecular Simulations	10
8	Computational approaches to select problems in molecule and material design	4
9	Project presentations/Discussions	3
10		
11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
3		
4		
5		
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7		
8		
9		
10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Gasteiger, J., Engel, T., Chemoinformatics, Wiley-VCH, 2008
2. Cramer, C.J., Essentials of Computational Chemistry, 2nd Ed., John Wiley & Sons Ltd., 2004.
3. Leach, A. R., Molecular Modelling: Principles and Applications, Longman, 1996.
4. D. Frenkel and B. Smit, Understanding Molecular Simulations: From Algorithms to Applications, Second Edition, Academic Press, 2002.
5 . M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids, Oxford University Press, 1987.

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	Open source softwares
19.2	Hardware	CSC computing resources
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	CHEMISTRY
2.	**Course Title** *(< 45 characters)*	MATERIALS CHARACTERIZATION
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL729
6.	**Status** (*category* for *program*)	Program Core

7.	**Pre-requisites** (course no./title)	Nil

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	Nil
8.2	Overlap with any UG/PG course of other Dept./Centre	Nil
8.3	Supercedes any existing course	Existing CYL729

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☐1st sem ☒2nd sem ☐Either sem

11.	**Faculty who will teach the course** Sameer Sapra, A Ramanan, Pravin P. Ingole	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)*: To introduce analytical techniques to probe structure, composition and phase transformation of solid materials
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)*: Compositional analysis of solid materials by X-ray and electron microscopic techniques. Basic concepts of diffraction techniques (powder and single crystal) in elucidating the crystal structures organic, inorganic and hybrid materials. Applications of electron microscopic techniques (scanning and transmission) for morphological and nanostructural features. Thermal analytical methods for correlating structural information and monitoring phase transition. Emphasis will be placed on the above techniques for industrially important materials and the interpretation and evaluation of the results obtained by various methods.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	X-ray spectroscopic methods (XAS, XRF and EDAX) for compositional analysis of solid materials	5
2	Basic concepts of diffraction techniques (powder & single crystal)	15
3	Electron microscopic techniques (SEM and TEM)	10
4	Scanning probe microscopy techniues: Scanning tunneling microscopy (STM), Atomic force microscopy (AFM) and Scanning electrochemical microscopy (SECM).	4
5	Thermal analysis: Thermal gravimetry analysis (TGA), Differential thermal analysis (DTA), Differential scanning calorimetry (DSC) and Dynamic mechanical analysis (DMA)	4
6	Photoemission spectroscopy (XPS, UPS, EELS, IPES)	4
7		
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10		
11		
12		
COURSE TOTAL *(14 times 'L')*		

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. V K Pecharsky and P Zavalij, Fundamentals of powder diffraction and structural characterization of materials, Springer (2005)
2. Wiliams, D.B.; Carter, C.B., Transmission Electron Microscopy – A Textbook for Materials Science, Plenum Press, New York (1996)
3. C. Richard Brundle, Charles A. Evans, Jr., and Shaun Wilson (Editors), Encyclopedia of Materials Characterization, Butterworth-Heinemann (1992)
4. J. Goldstein, D. Newbury, D. Joy, C. Lyman, P. Echlin, E. Lifshin, L. Sawyer, and J. Michael, Scanning Electron Microscopy and X-Ray Analysis (3rd Edition), Kluwer (2003)
5. J. A. Chandler, X-Ray Microanalysis in the Electron Microscopy (4th Edition), North

Holland (1987)
6. Ling Oii, Principle of X-ray crystallography, Oxford University Press (2008)
7. J. M. E. Walls (Editor), Methods of Surface Analysis: Techniques and Applications, Cambridge University Press (1990)
8. J. C. Riviere, Surface Analytical Techniques, Oxford University Press (1990)
9. D. P. Woodruff and T. A. Delchar, Modern Techniques of Surface Science, , Cambridge University Press (1994)
10. Haines, Laye, Principles of Thermal Analysis and Calorimetry; RSC Paperbacks, Volume 29 , Warrington

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	CHEMICAL SEPARATION AND ELECTROANALYTICAL METHODS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL731
6.	**Status** (*category* for *program*)	Program Core

7.	**Pre-requisites** (course no./title)	None

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	No
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	No

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☒1st sem ☐2nd sem ☐Either sem

11.	**Faculty who will teach the course** Pravin P Ingole, J D Singh, Nalin Pant	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)***:** The general objectives of this module is to explain the concepts underlying modern analytical techniques related to separation and electrochemical methods.

14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** Theory and applications of equilibrium and nonequilibrium separation techniques. Extraction, countercurrent distribution, gas chromatography, column and plane chromatographic techniques, electrophoresis, ultracentrifugation, and other separation methods, Modern analytical and separation techniques used in biochemical analysis. Principles of electro-chemical methods, electrochemical reactions, steady-state and potential step techniques; polarography, cyclic voltammetry, chrono methods, rotating disc and ring disc electrodes, concepts and applications of AC impedance techniques.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	General Concepts in Column Chromatography: Introduction, Family Tree of Chromatographic Methods, Zone Migration, Retention, Band Broadening, Resolution, Separation Time, Principles of Quantification	2
2	Gas Chromatography: Introduction, Mobile Phases, Stationary Phases, Retention in Gas-Liquid Chromatography, Preparation and Evaluation of Open Tubular Columns, Preparation and Evaluation of Packed Columns Instrumental Aspects of Gas Chromatography: Introduction, Pneumatic Systems, Thermal Zones, Sample Handling Devices, Sample Inlets, Supercritical Fluid Inlets, Vapor Sample Inlets, Coupled-Column Gas Chromatography, Column Connectors and Flow Splitters, Detector	3
3	Liquid Chromatography: Introduction, Column Packing Materials, Retention Mechanisms, Method Development, Column Preparation Instrumental Aspects of Liquid Chromatography: Introduction, Solvent Delivery Systems, Sample Inlets, Guard and Scavenger Columns, Column Temperature Control, Coupled-Column Systems, Detectors, Postcolumn Reaction Systems, Indirect Detection	3
4	Thin-Layer Chromatography: Introduction, Attributes of Layers and Columns, Theoretical Considerations, Stationary Phases, Sample Application, Multimodal (Coupled Column-Layer) Systems, Development Techniques, Method Development, Detection	3
5	Supercritical Fluid Chromatography: Introduction, Mobile Phases, Stationary Phases, Kinetic Optimization, Retention, Instrumental Aspects, Related Techniques	3
6	Capillary-Electromigration Separation Techniques: Introduction, Capillary Electrophoresis, Micellar Electrokinetic Chromatography, Capillary Electrochromatography, Capillary Gel Electrophoresis, Capillary Isoelectric Focusing, Capillary Isotachophoresis, Method Development, Instrumental Aspects	3
7	Separation of Stereoisomers: Introduction, Enantioselectivity and Absolute Configuration, Separation of Enantiomers, Chiral Stationary Phases, Chiral Mobile Phase Additives, Complexation Chromatography, Separation of Enantiomers as Covalent Diastereomer Derivatives, Liquid-Crystalline Stationary Phases	2
8	Laboratory-Scale Preparative Chromatography: Introduction, Thin-Layer Chromatography, Column Liquid Chromatography, Supercritical Fluid Chromatography, Gas Chromatography, Countercurrent Chromatography	2
9	Introduction and overview of electrode processes, Potentials and thermodynamics of cells, Kinetics of electrode reactions, Mass transfer by migration and diffusion.	6
10	Basic potential step methods, Potential sweep methods, Polarography and pulse voltammetry, Controlled-current techniques - chronoamperometry, chronocoulometry, chronopotentiometry.	5
11	Techniques based on concepts of Impedance, Bulk electrolysis methods, Electrode reactions with coupled homogeneous chemical reactions. Methods involving forced convection - Hydrodunamic methods.	6
12	Electrochemical instrumentation, Double layer structure and adsorption, Electroactive layers and modified electrodes,	4

	Photoelectrochemistry and spectro-electrochemistry	
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
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COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Douglas A. Skoog, F. James Holler, and Stanley R. Crouch, Principles of Instrumental Analysis, Brooks Cole; 6th edition 2006.
2. Georg Schewdt, The Essential Guide to Analytical Chemistry, John Wiley and Sons 2nd edition 1997.
3. Electrochemical Methods (Fundamentals and Applications), A.J.Bard ve L.R. Faulkner 2. Edition, John Wiley & Sons. Inc. New York
4. Analytical electrochemistry, Joseph WANG, 3. Edition, John Wiley & Sons. Inc. New York.

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	CHEMISTRY OF INDUSTRIAL CATAYSIS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL733
6.	**Status** (*category* for *program*)	Program elective

7.	**Pre-requisites** (course no./title)	None

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	No
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	CYL733

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☐1st sem ☐2nd sem ☒Either sem

11.	**Faculty who will teach the course** A Ramanan, N G Ramesh, Nalin Pant, A J Elias, V Haridas, J D Singh	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)*: Catalysis, be it heterogeneous or homogeneous, are ubiquitous in the chemical industry. This course presents the salient features of the chemistry behind the design and action of modern day catalysts.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)*: Fundamental aspects of Catalysis - Homogeneous & heterogeneous catalysis -The role of catalytic processes in modern chemical manufacturing - organometallic catalysts -catalysis in organic polymer chemistry -catalysis in petroleum industry - catalysis in environmental control.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Fundamental aspects of catalysis	10
2	Role of catalysis in manufacturing	6
3	Organometallic catalysts	10
4	Catalysts in polymer chemistry	6
5	Catalysis in petroleum industry	6
6	Catalysis in environmental control	4
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10		
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12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

Not Applicable

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
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COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Industrial Catalysis: A practical approach by Jens Hagen Wiley (2006)
2. Industrial Catalysis: Optimizing catalysts and processes by R. I. Wijngaarden, K. R. Westerterp, and A. Kronberg
3. Handbook of Industrial Catalysts by L. Lloyd
4. Fundamentals of Industrial Catalytic Processes by C. H. Bartholomew
5. Rothenberg, G., Catalysis: Concepts and green applications, Wiley VCH, 2008
6. Gupta, B. D, Elias, A. J., Basic Organometallic chemistry: Concepts syntheses and applications, 2nd edition, Orient Blackswan, 2013

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	Room with OHP and projector
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	CHEMISTRY OF NANOSTRUCTURED MATERIALS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL734
6.	**Status** (*category* for *program*)	Program elective

7.	**Pre-requisites** (course no./title)	None

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	No
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	CYL734

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☐1st sem ☐2nd sem ☒Either sem

11.	**Faculty who will teach the course** Pravin P Ingole, A Ramanan, S Sapra	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)***:** Chemistry has a paramount role in modern day materials science and people foresee that nanomaterials will revolutionize materials science. In this course the importance of chemistry in the directed synthesis of nanomaterials will be presented.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** Introduction; fundamentals of nanomaterials science, surface science for nanomaterials, colloidal chemistry; Synthesis, preparation and fabrication: chemical routes, self assembly methods, biomimetic and electrochemical approaches; Size controls properties (optical, electronic and magnetic properties of materials) - Applications (carbon nanotubes and nanoporous zeolites; Quantum Dots, basic ideas of nanodevices).

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Fundamentals of Nanomaterials: Introduction, quantum mechanics and atomic structure, Bonding and band structure,	5
2	surface energy, surface crystallography, surface reconfigurations, surface area and surface thrmodynamics, colloidal chemistry, nanoparticle nucleation and growth.	3
3	Synthesis and fabrication of Nanomaterials: coprecipitation, sol-gel process, microemulsions, hydrothermal methods, templated synthesis.	8
4	Self assembly: Hydrogen bonding -based assembly, electrostatic assembly, shape-selective assembly, hydrophobic assembly, collective properties of self assembled nanoparticles.	8
5	Biomimetic and electrochemical approached: Biomimetic nanotechnology, structural biomimicry, nanostructures in biodiagnostics and cell study, electrochemical methods of nanoparticles synthesis, anodic alumina oxide preparation, electrochemical deposition: constant current and constant potential.	3
6	Size controlled properties: Optical, electronic and magnetic properties of nanostructured materials.	8
7	Applications: Nanoelectronic materials, single electron transitors, single electron capacitors, quantum effects in transistors, carbon nanotube based electronic devices, spintronics,	7
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12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Fundamentals and Applications of Nanomaterials, Zhen guo & Li Tan, Artec House

publication.
2. The physics and chemistry of Nanosolids, Frank J. Owens & Charles P. Poole Jr., Wiley-Interscience publication.
3. Understanding Nanomaterials, Malkiat S. Johal, CRC Press (Taylor & Francis Group) publication.
4. Nanomaterials, B. Vishwanathan, Narosa Publishing house.

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	CHEMISTRY
2.	**Course Title** *(< 45 characters)*	APPLIED SPECTROSCOPY
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL737
6.	**Status** (*category* for *program*)	PROGRAM CORE

7.	**Pre-requisites** (course no./title)	NIL

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	15% with CYL566
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	No

9.	**Not allowed for** (indicate program names)	NIL

10.	**Frequency of offering**	☐ Every sem ☐ 1st sem ☒ 2nd sem ☐ Either sem

11.	**Faculty who will teach the course** Nalin Pant, N. G. Ramesh, V. Haridas, Nidhi Jain, R. P. Singh, S. Gholap, Ravi Shankar, S. Nagendran	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)*: This course aims to teach advanced level spectroscopic techniques, such as NMR and Mass spectrometry, for the structural determination of organic and inorganic compounds
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)*: Applications of advanced 1D-NMR techniques such as nOe, 1D 13C-NMR (including APT and DEPT) techniques, multinuclear NMR spectroscopy, 2D NMR techniques (COSY, HETCOR, HSQC, HMBC, NOESY, ROESY etc.) for the structural and stereochemical determination of organic compounds. Introduction to various types of ionizations (such as EI, CI, MALDI, field ionization/desorption, electrospray ionization) and analyzers (such as quadrupole, time of flight, triple quadupole, QqTOF, ion-trap) in mass spectrometry for MS, MS/MS and MSn applications. Determination of peptide sequencing using mass spectrometric techniques.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	1D NMR techniques (including nOe and 13C)	5
2	2D NMR techniques and their applications in the structural determination	10
3	Mass spectrometric techniques	7
4	Determination of peptide sequencing using mass spectrometry	5
5	Applications of combined mass and NMR techniques for strutural and stereochemical determination of organic compounds	7
6	Variable temperature NMR for studying stereochemical nonrigidity and fluxional behavior in inorganic and organometallic compounds	3
7	Multinuclear NMR spectroscopy (basic concepts and applications)	3
8	Hetreonuclear couplings and its applications in structural elucidation of inorganic/organometallic compounds	2
9		
10		
11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

NIL

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
3		
4		
5		
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7		
8		
9		
10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Silverstein R M, Webster F, Spectrometric Identification of Organic Compounds, 6th Edition, Wiley, 1998.
2. Simpson, J H., Organic Structure Determination using 2-D NMR Spectroscopy, 1st edition, Elsevier, 2008.
3. Gross J. H., Mass Spectrometry - A Text Book, 1st Edition, Springer, 2004.
4. Berger S, Sicker D., Classics in Spectroscopy - Isolation and Structural Elucidation of Natural Products, 1st Edition, Wiley, 2009.
5. Russell S. Drago, Physical methods in Inorganic Chemistry. 1st Edition, Van Nostrand Reinhold, 3rd Edition. 1994

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	NIL
19.2	Hardware	NIL
19.3	Teaching aides (videos, etc.)	NIL
19.4	Laboratory	NIL
19.5	Equipment	NMR AND MASS SPECTROMETERS ALREADY AVAILABLE IN THE INSTITUTE FOR DEMONSTRATION PURPOSE ONLY
19.6	Classroom infrastructure	OVERHEAD PROJECTOR
19.7	Site visits	No

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	NIL
20.2	Open-ended problems	NIL
20.3	Project-type activity	NIL
20.4	Open-ended laboratory work	NIL
20.5	Others (please specify)	NIL

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Department of Chemistry
2.	**Course Title** *(< 45 characters)*	APPLICATIONS OF P-BLOCK ELEMENTS AND THEIR COMPOUNDS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL738
6.	**Status** (*category* for *program*)	Program elective

7.	**Pre-requisites** (course no./title)	CYL 503 or equivalent for M.Sc students

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	CYL 668 Inorganic polymers (5% overlap)
8.2	Overlap with any UG/PG course of other Dept./Centre	nil
8.3	Supercedes any existing course	nil

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☐1st sem ☐2nd sem ☒Either sem

11.	**Faculty who will teach the course** S Nagendran, A J Elias, Ravi Shankar, J D Singh	
12.	**Will the course require any visiting faculty?**	No

13. Course objective *(about 50 words)*:

Unlike transition metals, elements of the p block and their compounds have a wide range of proven scientific and industrial applications as bulk materials, fertilizers, electronic and solar energy materials, pesticides, explosives, nuclear reactor materals, semiconductors, polymers such as silicones, framework aluminosilicates,zeolites, LED's and TCO and carbon based nano materials such as fullerenes, nanotubes and graphene.The course will not only focus on the synthesis and unique properties leading to the application potential of such compounds but also explore new developments in p block chemistry such as frustrated Lewis acid base pairs and low valent main group chemistry.

14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** Introduction, Structure, bonding and recent discussions on d orbital participation. Boranes, carboranes and metallaboranes and their use in BNCT and as control rods in nuclear reactors, modern electron counting methods such as Jemmis rules, chemistry of B(0) and B(1). GaAs, GaN, InSnO3: Synthesis and applications in solar cells, LED and as transparent conducting materials. Fullerenes, nanotubes, graphene, silicates, aluminosilicates, zeolites and their applications. Silicones and their industrial applications. Si(II) and Ge(II) chemistry. NHC's and their use in stabilizing main group compounds. Nitrogen based fertilizers, Ammonia, Haber-Bosch Process, nitrogen based explosives, hydrazines as rockel fuels, applications of azides and pentazenium. Phosphorus based fertilizer processes, phosphorus based pesticides, phosphorus-nitrogen compounds as multidentate ligands, superbases, dendrimer cores and polymers. Phosphines and their industrial uses. Frustrated Lewis acid bases as catalysts. Superacids and their uses. Sulphonamides, industrial applications of sulfur and selenium. Fluorine in pharmaceuticals, fluoropolymers.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Introduction; General and periodic properties of p block elements, structure & bonding,modern aspects on hydridization and orbital participation involving d orbitals	2
2	Properties of boron compounds, control rods, BNCT, Boranes as fuels, carboranes, macropolyhedral clusters and Jemmis rules, Chemistry of B(I) and B(0)	4
3	Properties of Al, Ga and In: GaAs solar cells, GaN and related LEDs, ITO as transparent conducting oxides, Al(I) and Ga(I) chemistry	5
4	Properties of carbon and silicon: fullerenes, nanotubes, graphene, silicates, aluminosilicates zeolites and their applications	6
5	Synthesis of silicones and their industrial applications. Si(II), Ge(II) chemistry. classification of NHC's and their use in stabilizing low valent main group compounds. Germanium-infra red detector applications	4
6	Properties of nitrogen compounds applications in fertilizers, Ammonia, Haber Bosch Process, nitrogen based explosives, hydrazines as rockel fuels, synthesis and applications of azides and pentazenium	6
7	Phosphorus based fertilizer processes, phosphorus based pesticides, chemistry and activity , phosphorus nitrogen compounds, multidentae ligands, superbases, dendrimer cores and polymers, ATP and related chemistry, Phosphines and their indsutrail uses. Frustrated Lewis acid base pairs and applications	6
8	Arsenic and antimony based compounds- superacids and their uses	2
9	Properties of sulfur, selenium and tellurium: sulphonamides, industrial applicatios of sulfur compounds, biologialy important compounds such selenocysteine and glutathione peroxidase, new selenium and tellurium based ligands and their uses	4
10	Properties of halogen compounds. Fluorine in pharmaceuticals, fluoropolymers and their properties, teflon and CFC. Industrial uses of chlorine and its compounds	3
11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

No tutorials are required

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1	NA	
2		
3		
4		
5		
6		
7		
8		
9		

10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Henderson, W., Main Group Chemistry, RSC 2003
2. Akiba K., Organo Main group Chemistry, Wiley 2011
3. Green wood N.N, Earnshaw L., Chemistry of the elements 2nd edn, ELsevier 1997
4. Chivers T and Manners I., Inorganic rings and polymers of the p block elements, RSC 2009
5. Ullmanns encyclopedia of Industrial chemistry (selected chapters on silicon, phosphorus and fluorine
6. Roesky P. W Compounds with low-valent group 13 metals as ligands for electron poor main group and transition metals. Dalton Trans, 2009, 1887
7. L.J. Hounjet, D.W. Stephan, Hydrogenations by Frustrated Lewis Pairs: Main Group Alternatives to Transition Metal Catalysts, Organic Process Research & Development, 2014, 18, 384-391.

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	Class-room with projector
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	APPLIED BIOCATALYSIS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL739/CYL695
6.	**Status** (*category* for *program*)	Program elective

7.	**Pre-requisites** (course no./title)	Nil

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	Same course is already running as CYL695 as PE for M.Sc/M.Tech in the Department
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	No

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☐1st sem ☐2nd sem ☒Either sem

11.	**Faculty who will teach the course** S K Khare, Tanmay Dutta	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)*: This course aims at educating the students about enzymes and biocatalysis with their applications in various industrial processes.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)*: Introduction to enzymes and enzyme catalysed reactions. Classification and mechanism of reaction. Purification and characterization of enzymes. Michelis Menten kinetics, Industrial enzymes. Applications of enzymes in diagnostics, analysis, biosensors and other industrial processes and bio-transformations.Enzyme structure determination, stability and stabilisation. Enzyme immobilization and concept of enzyme engineering. Nanobiocatalysis.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Introduction to enzymes.	3
2	Enzyme catalysed reactions.	4
3	Classification and mechanism of reaction	3
4	Purificarion and characterisation of enzymes	3
5	Michaelis menten kinetics	3
6	Industrial enzymes	3
7	Applications of enzymes in diagnostics, analysis, biosensors and other industrial processes.	5
8	Bio-transformations	3
9	Enzyme structure determination	4
10	Stability and stabilization	3
11	Enzyme immobilization and the concept of enzyme engineering	4
12	Nanobiocatalysis	4
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Price and Stevens, Fundamentals of enzymology, Oxford University Press
2. Buchholz, Kasche and Bornscheuer, Biocatalysts and Enzyme Technology, Wiley
3. Polaina and MacCabe, Industrial Enzymes: Structure, Function and Applications, Springer

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	Enzo
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	

19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	Projector
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	CHEMISTRY OF HETEROCYCLIC COMPOUNDS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL740
6.	**Status** (*category* for *program*)	Program elective

7.	**Pre-requisites** (course no./title)	None

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	Same course is floated as CYL675 as Departmental elective for M.Sc. students
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	Nil

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☐1st sem ☐2nd sem ☒Either sem

11.	**Faculty who will teach the course** Nalin Pant, N G Ramesh, V Haridas, Nidhi Jain, Ravi P Singh, Shivaji Gholap,	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)***:** Heterocyclic compounds are present in a number of natural products that are of biological significance. This course covers the various aspects of heterocyclic chemistry.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** Chemistry of heterocyclic compounds containing one, two and three heteroatoms. Total synthesis of representative natural products.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Introduction to heterocyclic chemistry	5
2	Chemistry of heterocyclic compounds containing one heteroatom	5
3	Chemistry of heterocyclic compounds containing two heteroatoms	5
4	Chemistry of eterocyclic compounds containing three heteroatoms	5
5	Complex naturally occurring heterocylic systems	5
6	Total syntheis of representative natural products	17
7		
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10		
11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

No

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. T. L. Gilchrist, "Heterocyclic Chemistry", John Wiley & Sons.
2. A. R. Katritzky, "Hand Book of Heterocyclic Chemistry", Academic Press.

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	

19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	ORGANO AND ORGANOMETALLIC CATALYSIS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL741
6.	**Status** (*category* for *program*)	PROGRAM ELECTIVE

7.	**Pre-requisites** (course no./title)	Nil

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	5% with CYL562
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	No

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐Every sem ☐1st sem ☐2nd sem ☒Either sem

11.	**Faculty who will teach the course** N Pant, N G Ramesh, V Haridas, Nidhi Jain, Ravi P Singh, Shivaji Gholap	
12.	**Will the course require any visiting faculty?**	NA

13.	**Course objective** *(about 50 words)*: Operationally, enzymes are the most effective catalyst around. In mimmicing it, chemist always try to design a system which is more closer in function and structure to it. In this course the frontiers in catalysis will be discussed.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)*: Introduction. Enamine catalysis. Iminium catalysis. Asymmetric proton catalysis. Ammonium ions as chiral templates. Chiral Lewis bases as catalysts. Asymmetric acyl transfer reactions. Ylide based reactions. Transition metal catalyzed reactions. C-H activation. N-Heterocyclic carbenes.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Introduction. Enamine catalysis: Aldol and Mannich type reactions, α-heteroatom functionalization, direct conjugate additions via enamine activation. Iminium catalysis: the catalysis concept, cycloaddition reactions, 1,4-addition reactions, transfer hydrogen,cascade reactions.	4
2	Addition of ketones and aldehydes to activated olefins (MBH), asymmetric MBH reactions. Asymmetric proton catalysis: conjugate addition reactions, hydrocyanation reactions, Mannich reactions, aza-Henry reaction, acyl Pictet-Spengler reaction, aza Friedel-Crafts reaction.	4
3	Ammonium ions as chiral templates: Homogeneous catalysis with chiral quaternary ammonium salts, Heterogeneous catalysis- chiral phase transfer catalysis.	4
4	Chiral Lewis bases as catalysts: allylation reactions, propargylation reactions, hydrocyanation and isonitrile addition, aldol type reactions, reduction of imines, epoxide ring opening.	4
5	Asymmetric acyl transfer reactions. Nucleophilic N-Heterocyclic carbenes (NHCs) and their application in organic synthesis	8
6	Ylide based reactions. Organocatalytic oxidation and reduction reactions	4
7	Fundamental reaction steps of transition metal catalysed reaction. Coordinative unsaturation , oxidative-addition, elimination reactions, cleavage of C-H bonds, activation of sulphur hetrocycles, migration reaction, insertion reaction	6
8	C-H Activation: Introduction, Metal or Non-metal based activation, sp3 C-H and sp2 C-H activation, Application for functionalization: intramolecular and intermolecular version (Pd, Cu, Rh)	8
9		
10		
11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
3		
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10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Asymmetric Organocatalysis – From Biomimetic Concepts to Applications in Asymmetric Synthesis By A. Berkessel and H. Groger. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2005.
2. Enantioselective Organocatalysis: Reactions and Experimental Procedures Edited by Peter I. Dalko Publisher: Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2007.
3. Organocatalysis Reetz, M.T.; List, B.; Jaroch, S.; Weinmann, H. (Eds.) Series: Ernst Schering Foundation Symposium Proceedings 2007-2 , Publisher: Springer-Verlag, Berlin Heidelberg, 2008.
4. Advanced Inorganic Chemistry F.A Cotton 6th addition chapter 21 and 22, p. 1167-1294
5. Stereoselective Organiocatalysts - Torrres, R. R., 1st Edition, WILEY, 2013.

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	REAGENTS IN SYNTHETIC TRANSFORMATIONS
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL742
6.	**Status** (*category* for *program*)	Program elective

7.	**Pre-requisites** (course no./title)	None

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	25% with CYL562
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	No

9.	**Not allowed for** (indicate program names)	Not applicable

10.	**Frequency of offering**	☐Every sem ☐1st sem ☐2nd sem ☒Either sem

11.	**Faculty who will teach the course** N Pant. N G Ramesh, V Haridas, Nidhi Jain, Ravi P Singh, Shivaji Gholap	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)*: To introduce students with the state-of-the-art of the reagents.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)*: The course will cover the applications of various oxidation and reduction reactions in organic chmeistry with s[pecial emphasis on special reagents that are used for selective transformations. Use of organolithium and organoboron compoinds in organic synthesis and olefin metathesis will also serve a part of the course.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Advance Oxidising Reagents - Metal based oxidizing reagents: Chromium, Manganese, Ruthenium, Silver, Osmium, Kharasch-Sosnovsky Reaction, Sharpless Asymmetric Epoxidation and Dihydroxilation, Saegusa Oxidation	4
2	Advance Non-Metal based oxidizing reagents: DMSO, peroxide, IBX, DMP, CAN, DDQ and Periodate, Shi Epoxidation, Enolate Oxidation: Via selenoxide elemination, Via Dehydrogenation with IBX, With Oxaziridines; Baeyer-Villiger Oxidation, Tamao oxidation	8
3	Advance Reducing Reagents- Homogeneous and heterogeneous hydrogenation, Borane based racemic and chiral reagents for reduction, Aluminum, Tin, Silicon based reducing agents, Dissloving metal reductions, Asymmetric Rhodium catalysed hydrogenation, Luche Reduction, Sandoz Reduction, Evans Me4NBH(OAc)3 anti-selective hydroxyl directed reduction, Super hydride and the Selectride, Evans-Tischenko Reduction, Alpine-borane reduction, CBS reduction, Asymmetric catalytic transfer hydrogenation of ketone, Shapiro reaction	9
4	Organolithium Reagents: Preparation of organolithium reagents by reductive metallation, halogen based exchange, Shapiro reaction, Retention versus inversion of configuration in their reactions and the importance of HSAB principle	5
5	Organoboron reagents: Preparation, Use in functional group interconversions, Allylboranes, preparation and reactivity with aldehyde including diastereoselective and enantiospecific reactions, Carbon-carbon bond formation by Michael addition/radical formation and carbonylation reactions	7
6	Alkene metathesis and related reactions: Grubb's Catalyst, Ring opening metathesis polymerisation, Ring closing metathesis, Cross metathesis, Enyne metathesis, Alkyne metathesis	5
7	Miscellaneous Reagents: N-Bromosuccinimide (NBS), N,N-Dicyclohexylcarbodiimide (DCC), Diazomethane	4
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11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1		
2		
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4		
5		

6		
7		
8		
9		
10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. W. Carruthers and I. Coldham, Modern Methods of Organic Synthesis, 4th ed., Cambridge University Press, UK, 2004.
2. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Part A & B, 5th ed., Springer, New York, 2007.
3.J. March, Advanced Organic Chemistry, 4th ed., John Wiley & Sons, Inc., Canada, 1992
4. Herbert O. House, Modern Synthetic Reactions, Second ed.

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	CHEMISTRY
2.	**Course Title** *(< 45 characters)*	MOLECULAR MODELING AND SIMULATIONS: CONCEPTS AND TECHNIQUES
3.	**L-T-P structure**	3-0-0
4.	**Credits**	3
5.	**Course number**	CYL801
6.	**Status** (*category* for *program*)	Program elective

7.	**Pre-requisites** (course no./title)	None

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	CYL668 and CYL726 provide introductions to this and allied topics. This is a follow-up course for those interested in doing research in this area.
8.2	Overlap with any UG/PG course of other Dept./Centre	Simulation and statistical mechanics courses have been offered by the departments of chemistry, physics and chemical engineering at various levels. To our knowledge, no course exists in IIT-Delhi at the pre-Ph.D. level The coverage of topics and the orientation will reflect the connection with various areas of chemical sciences and will complement existing courses and allow the students to acquire a grasp of advanced research

		techniques.
8.3	Supercedes any existing course	No

9.	**Not allowed for** (indicate program names)	

10.	**Frequency of offering**	☐Every sem ☐1st sem ☐2nd sem ☒Either sem

11.	**Faculty who will teach the course:** Charusita Chakravarty, Hemant Kashyap and B. Jayaram	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)***:** Molecular simulations complement theory and experiment in many areas of chemistry, condensed matter physics, chemical engineering, materials science and biology. The purpose of this course is to provide students with an understanding of the conceptual basis as well as familiarity with molecular simulation methods so that they can use them effectively in their research,

14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** I. Review of Basic Concepts: Length and Time Scales, Intermolecular Interactions and Potential Energy Surfaces, Evaluation of Long-range interactions II. Static and Dynamic Properties of Simple and Complex Liquids III. Molecular Dynamics: Microcanonical and other ensembles; Constrained simulations; non-equilibrium approaches IV. Monte Carlo Methods: Random Numbers and Random Walks , Metropolis Algorithm in various ensembles, Biased Monte Carlo Schemes V. Free Energy Estimations: Mapping Phase Diagrams, Generating Free Energy Landscapes, Collective Variables VI. Rare Event Simulations and Reaction Dynamics VII. Advanced Topics: First principles molecular dynamics, Quantum Monte Carlo methods, Coarse-Graining and Multiscale Simulations for Nanoscale Systems, Quantum mechanics/molecular mechanics (QM/MM) approaches. (To some extent, coverage of advanced topics will depend on research interests of students and faculty since this is a Pre-Ph.D. course)

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1	Review of Basic Concepts	3
2	Static and Dynamic Properties of Simple and Complex Liquids	6

3	Molecular Dynamics	6
4	Monte Carlo	6
5	Free energy estimations	6
6	Rare Event Simulations and Reaction Dynamics	6
7	Advanced Topics	9
8		
9		
10		
11		
12		
COURSE TOTAL *(14 times 'L')*		42

16. Brief description of tutorial activities: Not applicable

17. Brief description of laboratory activities: Not applicable

Module no.	Experiment description	No. of hours
1		
2		
3		
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7		
8		
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10		
COURSE TOTAL *(14 times 'P')*		

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. M. E. Tuckerman, Statistical Mechanics: Theory and Molecular Simulations (Oxford University Press)
2. D. Frenkel and B. Smit, Understanding Molecular Simulations: From Algorithms to Applications
3. M. P. Allen and D. J. Tildesley, Computer Simulation of Liquids
4. Andrew R. Leach, Molecular Modeling: Principles and Applications
5. C. Chipot and A. Pohorille, Editors. Free Energy Calculations: Theory and Applications in Chemistry and Biology

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	Public domain software
19.2	Hardware	Access to Computer Service Centre facilities
19.3	Teaching aides (videos, etc.)	

19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	Overhead projection/Internet connectivity
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	We expect that 25-30% of student time will be spent on a project that implements the techniques discussed in the course for a system of interest from the point of view of their research and ensure appropriate coverage of applications, including those related to materials science and biomolecular systems.
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	Chemistry
2.	**Course Title** *(< 45 characters)*	SYNTHESIS OF ORGANIC AND INORGANIC COMPOUNDS
3.	**L-T-P structure**	0-0-6
4.	**Credits**	3
5.	**Course number**	CYP722
6.	**Status** (*category* for *program*)	Program core

7.	**Pre-requisites** (course no./title)	Only for students of this M.Tech Program

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	No
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	CYP722

9.	**Not allowed for** (indicate program names)	Nil

10.	**Frequency of offering**	☐ Every sem ☒ 1st sem ☐ 2nd sem ☐ Either sem

11.	**Faculty who will teach the course** Nalin Pant, N G Ramesh, V Haridas, Nidhi Jain, Ravi P Singh, Shivaji Gholap, J D Singh, S Nagendran, Ravi Shankar	
12.	**Will the course require any visiting faculty?**	No

13.	**Course objective** *(about 50 words)***:** The main objectives are to give hands-on experience in performing various experiments through synthesis of organic compounds (single, double and multi stage synthesis), organometallic compounds and inorganic materials and to characterize them using IR, UV, mass and 1H-NMR spectroscopic techniques.
14.	**Course contents** *(about 100 words) (Include laboratory/design activities)***:** Single, double and multi-stage preparation of organic, inorganic and organometallic compounds; experiments involving the concepts of protecting groups and selectivity; identification of compounds through thin-layer chromatography and their purification by column chromatography. Characterization of synthesized compounds using IR, UV, 1H-NMR and mass spectromteric techniques.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1		
2		
3		
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6		
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11		
12		
COURSE TOTAL *(14 times 'L')*		

16. Brief description of tutorial activities

Not Applicable

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1	Single step synthesis of organic compounds	12
2	Two step synthesis of organic compounds	12
3	Multi-step synthesis of organic compounds	18
4	Experiemts based on protecting groups	12
5	Synthesis of inorganic complexes	12
6	Synthesis of materials	12
7	Application of organometallic compounds insynthesis	6
8		
9		
10		
COURSE TOTAL *(14 times 'P')*		84

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

Lab manual containing various experiments will be provided to the students.

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	
19.4	Laboratory	
19.5	Equipment	General laboratory equipments for performing the experiments.
19.6	Classroom infrastructure	

19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)

COURSE TEMPLATE

1.	**Department/Centre proposing the course**	CHEMISTRY
2.	**Course Title** *(< 45 characters)*	INSTRUMENTATION LABORATORY
3.	**L-T-P structure**	0-0-6
4.	**Credits**	3
5.	**Course number**	CYP728
6.	**Status** (*category* for *program*)	Program core

7.	**Pre-requisites** (course no./title)	Only for M.Tech students of this program

8.	**Status vis-à-vis other courses** *(give course number/title)*	
8.1	Overlap with any UG/PG course of the Dept./Centre	No
8.2	Overlap with any UG/PG course of other Dept./Centre	No
8.3	Supercedes any existing course	CYP728

9.	**Not allowed for** (indicate program names)	Students from other Departments and other programs

10.	**Frequency of offering**	☐ Every sem ☐ 1st sem ☒ 2nd sem ☐ Either sem

11.	**Faculty who will teach the course** N D Kurur, S Pandey, P K Chaudhury, S Deep, S Sapra	
12.	**Will the course require any visiting faculty?**	NO

13.	**Course objective** *(about 50 words)*: Introduce students to various advanced spectroscopic instrumental methods commonly used in characterizing molecules.

14.	**Course contents** *(about 100 words) (Include laboratory/design activities)*: Experiments based on Instrumental methods of chemical analysis involving spectroscopy, microscopy and thermal methods.

15. Lecture Outline *(with topics and number of lectures)*

Module no.	Topic	No. of hours
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
11		
12		
COURSE TOTAL *(14 times 'L')*		

16. Brief description of tutorial activities

17. Brief description of laboratory activities

Module no.	Experiment description	No. of hours
1	UV-Vis spectroscopy (Particle-in-a-box, can include quantum dots or any other)	6
2	Atomic Absorption Spectroscopy for trace metal detection	6
3	Circular Dichroism Spectroscopy for Protein Structure Elucidation	6
4	FTIR spectroscopy (need a benchtop FTIR spectrometer)	6
5	Fluorescence spectroscopy (steady-state and time resolved; for the latter we will need to buy a basic fluorescence lifetime system)	6
6	Raman spectroscopy (we are in the process of purchasing a portable Raman spectrometer)	6
7	Experiments based on NMR spectroscopy	30
8	DSC to obtain phase transitions	6
9	GC-MS for the analysis of volatiles	6
10	HPLC in separation science	6
COURSE TOTAL *(14 times 'P')*		84

18. Suggested texts and reference materials

STYLE: Author name and initials, Title, Edition, Publisher, Year.

1. Experiments in Physical Chemistry by C. W. Garland, J. W. Nibler and D. P. Shoemaker.
2. S. Berger and S. Braun, 200 and more NMR experiments, Wiley-VCH, Weinheim, 2004

19. Resources required for the course *(itemized & student access requirements, if any)*

19.1	Software	
19.2	Hardware	
19.3	Teaching aides (videos, etc.)	

19.4	Laboratory	
19.5	Equipment	
19.6	Classroom infrastructure	
19.7	Site visits	

20. Design content of the course *(Percent of student time with examples, if possible)*

20.1	Design-type problems	
20.2	Open-ended problems	
20.3	Project-type activity	
20.4	Open-ended laboratory work	
20.5	Others (please specify)	

Date: (Signature of the Head of the Department)