Course Structure and Detailed Syllabi Ph.D.

(Chemistry)

(Revised)

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Department of Chemical Sciences

(DST-FIST and UGC-SAP DRS-II SUPPORTED)

TEZPUR UNIVERSITY

YAER 2020

Preamble

The curriculum content of Ph.D. in Chemical Sciences is designed to learn approach of research methodology, identification of new research opportunities, plan effective strategies for pursuing these opportunities, and conduct research that contributes in a meaningful way to current knowledge in the chosen sub discipline of chemistry or related areas. It also provides student knowledge based necessary skills to become productive, ethical, and independent scientists.

1. Introduction

The main objectives of Ph.D. in Chemistry programme is to prepare quality doctorates for further research and development and entrepreneurship through participation in world-class research and to impart the knowledge of chemical sciences to the different stakeholders of society. The programme offers course work to the students in the initial two year period to enlighten them with the methodology, problem solving skills and techniques involved in current research trends. The credit requirement to complete the course work is minimum 16 credits. The eligibility criteria for enrolment in the PhD programme is M.Sc. in all branches of Chemical Science/Physics/Nanoscience/ Material Science/ Biotechnology/ Biochemistry/ Bioinformatics/ Environmental Science. Furthermore, students having M.E./M.Tech. in allied subjects (Chemical Engineering/ Polymer Technology/ Material Sciences/ Environmental Engineering etc. are also eligible for the programme.

2. Qualification descriptors for the graduates

Knowledge & Understanding:

- Ability to apply concepts and principles of chemistry in chemical science research and in interdisciplinary scenarios.
- Acquisition of competence in the use of routine materials, techniques and practices of chemistry.
- Demonstrations of skills in the use of safety data sheet, safe handling of chemical materials considering their physical and chemical properties including any specific hazards associated with their use and disposal by minimizing the environmental impact.

Skills and Techniques:

- Maintaining of ethics in the presentation of experimental data and result, and the standard related to plagiarism.

- Development of awareness of the role of chemistry in contemporary societal and global issues, including areas such as Energy crisis, pollution, sustainability and green chemistry.

Competence:

- Development of competence in intellectual, practical and transferable skills (Communication skills, IT skills, societal skills) necessary for employment as professional chemist.
- Able to choose research as professional career.
- Development of competence in addressing different problems associated with society and environment.

3. Graduate Attributes

- Ph.D. doctorate of this program will earn necessary skills to become productive, ethical, and independent researcher
- Research scholars will acquire knowledge based ability to identify innovative research opportunities, effective strategies for execution of research objectives to related fields of Chemistry

4. Program Outcomes

PO1. Graduates of this program will demonstrate the necessary skills to become productive, ethical, and independent scientists.

PO2. Program graduates will understand and critically evaluate current research in their chosen subdiscipline in chemistry.

PO3. Coursework that builds upon the student's undergraduate and postgraduate education and excessive literature survey in the first two semester will provide the initial steps to achieve this outcome.

PO4. Program graduates will demonstrate proficiency in laboratory techniques necessary to contribute to knowledge in their chosen subdiscipline of chemistry.

PO5. Research scholars will learn to effectively write scientific manuscripts describing their research and to make oral presentations of their research at scientific meetings.

5. Programme Structure

Course category	No. of courses	Credits per course	Total Credits
I. Core	2	2/4	6
II. Elective*	2	4	8
III. CBCT	1	4	4
Total Credits			18

*** Students can take any two courses from the list of elective mentioned below**

6. Course structure

Course type	Course title	Lecture (L)	Tutorial (T)	Practical (P)	Contact Hours (CH)	Credits
Core	CH-712: Research Methodology	4	0	0	4	4
	RP 799: Research and Publication Ethics	1	0	1	3	2
CBCT	CBCT	4	0	0	4	4
Elective	CH-713: Applications of Spectroscopic Tools	3	1	0	4	4

	CH-714: Petrochemicals	3	1	0	4	4
	CH-715: Advanced Instrumental Methods in Chemistry	2	0	2	6	4
	CH-716: Green Chemistry	2	2	0	4	4
	CH-717: Computational Chemistry	2	2	0	4	4
	CH-718: Nature and Applications of Surfactants	2	0	2	6	4
	CH-719: Chemistry of Bioactive Molecules	3	1	0	4	4
	CH-720: Density Functional Theory	2	0	2	4	4
	CH-721: Dendritic Polymers	3	1	0	4	4
	CH- 722: Polymeric Nanocomposites	3	1	0	4	4
	CH-723: High Performance Polymers	3	1	0	4	4
	CH-724: Polymeric Biomaterials	3	1	0	4	4
	CH-725: Catalytic Chemistry	3	1	0	4	4

7. Mapping of course with programme outcome (POs)

Course Title	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**
CH-712: Research Methodology	✓	✓			✓
RP 799: Research and Publication Ethics	✓	✓	✓	✓	✓
CH-713: Applications of Spectroscopic Tools	✓	✓	✓	✓	✓
CH-714: Petrochemicals			✓	✓	

CH-715: Advanced Instrumental Methods in Chemistry	✓	✓	✓	✓	
CH-716: Green Chemistry	✓	✓	✓	✓	
CH-717: Computational Chemistry		✓	✓	✓	
CH-718: Nature and Applications of Surfactants		✓	✓	✓	
CH-719: Chemistry of Bioactive Molecules		✓	✓	✓	
CH-720: Density Functional Theory		✓	✓	✓	
CH-721: Dendritic Polymers		✓	✓	✓	
CH- 722: Polymeric Nanocomposites		✓	✓	✓	
CH-723: High Performance Polymers		✓	✓	✓	
CH-724: Polymeric Biomaterials		✓	✓	✓	
CH-725: Catalytic Chemistry	✓	✓	✓	✓	

8. Evaluation plan

Students will be evaluated as per academic rules of Tezpur University.

9. Detailed Syllabus

CH 712 Research Methodology L 2 T 0 P 2 CR 4

Course outcomes:

On completion of this course the students will be able to learn:

CO1: Application of a number of principles as applied to chemical research

CO2: Design, conduct, analyse and interpret results of an experiment, and effectively communicate these in written reports

CO3: Critical analysis and evaluation of quantitative & qualitative chemical information

CO4: Obtain and evaluate information from a variety of sources

CO5: Extend knowledge and understanding of a variety of chemical concepts in a range of contexts

Course Contents:

Introduction to Research Methodology [8 Lectures]

Research Methodology: An Introduction Objectives of Research, Types of Research, defining a Research Problem, Techniques involved in Defining a Problem Research Design Technical Writing, Ethics in Research, Software for Plagiarism.

Error Analysis [4 Lectures]

Instrumental and statistical uncertainties, propagation of errors, specific error formulae, application of error equation.

Hypothesis and Research Methodology [12 Lectures]

Basic Principles of Experimental Designs and Sampling, Methods of Data Collection and Analysis Collection of Primary and Secondary Data, Selection of appropriate method Data Processing Operations, Elements of Analysis, Statistics in Research, Regression Analysis, Correlation Techniques of Hypotheses, Parametric or Standard Tests Basic concepts.

Computational Techniques [5 Lectures]

Analysis of Variance and Co-variance ANOVA, One way ANOVA, Two Way ANOVA, ANOCOVA Assumptions in ANOCOVA. Basics of computational chemistry.

Seminar **[7 Lectures]**

Seminar presentation

Text Books:

1. C. R. Kothari, "Research Methodology", 2nd Ed. Wiley Eastern, New Delhi, 1985.

2. Ranjit Kumar, "Research Methodology-A step by step guide for beginners", 2nd Ed. Pearson Education, 2005.

Reference Book

1. John W Best, V. Kahn, *"Research in Education", 8th Ed. PHI Publication,* 1998.

2. K.N. Krishna swami and others, *"Management Research Methodology-Integration of principles, methods and Techniques", 1st Ed. Pearson Education,* 2009.

RP 799 Research and Publication Ethics L 1 T 0 P1 CR 2

Course outcomes:

On completion of this course the students will be able to learn:

CO1: Basics of philosophy of science and ethics, research integrity, publication ethics
CO2: Identification of research misconduct and predatory publications
CO3: Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor, etc.)
CO4: Plagiarism tools and their use
CO5: Communication of research finding without ethical violation

Course Contents:

THEORY

RPE 01: PHILOSOPHY AND ETHICS (3 hrs.) [3 Lectures]

1. Introduction to philosophy: definition, nature and scope, concept, branches
2. Ethics: definition, moral philosophy, nature of moral judgements and reactions

RPE 02: SCIENTIFICCONDUCT [5 Lectures]

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: Falsification, Fabrication, and Plagiarism (FFP)
4. Redundant publications: duplicate and overlapping publications, salami slicing
5. Selective reporting and misrepresentation of data

RPE 03: PUBLICATION ETHICS [7 Lectures]

1. Publication ethics: definition, introduction and importance
2. Best practices / standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behavior and vice versa, types
5. Violation of publication ethics, authorship and contributorship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

PRACTICE

RPE 04: OPEN ACCESS PUBLISHING [4 Lectures]

1. Open access publications and initiatives
2. SHERPA/RoME0 online resource to check publisher copyright & self-archiving policies
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder / journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

RPE 05: PUBLICATION MISCONDUCT [4 Lectures]

A. Group Discussions (2 hrs.)

1. Subject specific ethical issues, FFP, authorship

2. Conflicts of interest

3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools (2 hrs.)

Use of plagiarism software like Turnitin, Urkund and other open source software tools

RPE 06: DATABASES AND RESEARCH METRICS [7 Lectures]

A. Databases (4 hrs.)

1. Indexing databases
2. Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs.)

1. Impact Factor of journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score
2. Metrics: h-index, g index, il 0 index, altmetrics

Reference Books:

1. A. Bird, Philosophy of Science, Routledge, 2006.
2. A. MacIrityre, A Short History of Ethics, London, 1967
3. P. Chaddah, Ethics in Competitive Research: Do not get scooped; do not get plagiarized, 2018. ISBN:978-9387480865
4. National Academy of Sciences, National Academy of Engineering and Institute of Medicine. On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition. National Academies Press., 2009.
5. D. B. Resnik, What is ethics in research & why is it important. National Institute of Environmental Health Sciences, 1-10, 2011. Retrieved from https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm
6. J. Beall, Predatory publishers are corrupting open access. Nature, 489(7415), 2012, 179-179. https://doi.org/10.1038/489179a
7. Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance(2019), ISBN:978-81-939482-1-7. http://www.insaindiaxes.in/pdf/Ethics Book.pdf

CH-713 Application of Spectroscopic Tools L 3 T 1 P 0 CR 4

Course Outcomes:

On completion of this course the students will be able to understand:

CO1: Basic principles of spectroscopy, interaction of electromagnetic radiation with matter, atomic and molecular spectroscopy and the chemical structure-spectral property relationship.
CO2: Basic principles and instrumentation of various spectroscopic techniques viz FTIR, Raman, UV-vis, NMR including 2D, ESR, and Mass spectrometry
CO3: Application of the spectroscopic techniques in predicting the functional groups, structure of organic and inorganic compounds, paramagnetic behaviour, geometrical parameters like bond length, bond angles etc.
CO4: Hands on experience of different spectroscopic tools and the software for analysing data.

Course Contents:

Infrared and Raman Spectroscopy: **[5 Lectures]**

Structural studies (involving IR and Raman spectroscopy) of coordination and organometallic compounds. Structure elucidation of organic compounds by IR spectroscopy.

Fluorescence Spectroscopy: **[7 Lectures]**

Basic principles**,** Fluorescence sensing: Mechanism of sensing; sensing techniques based on (i) collisional quenching, (ii) energy transfer, (iii)electron transfer; examples of (i) pH sensors, (ii) glucose sensors & (iii) protein sensors. Novel fluorophores: (i) quantum dots, (ii) lanthanides and (iii) long-lifetime metal-ligand complex.

Magnetic Resonance Spectroscopy **[5 Lectures]**

Electron spin resonance spectroscopy: Evaluation of g values and metal hyperfine coupling constants. ESR spectroscopy of Cu, V, Mn and Fe metal complexes, organic free radicals. Application of ESR spectroscopy in bioinorganic systems.

Nuclear magnetic resonance spectroscopy: **[5 Lectures]**

Chemical shift (aliphatic, olefinic, alkynes, aromatic, hetero-aromatic, carbonyl carbon); Coupling constants, two-dimensional NMR spectroscopy, NOESY, DEPT and INEPT terminologies. Applications of ^{31}P, ^{19}F, spectroscopy in the structural assessment of inorganic compounds

Mass Spectroscopy: **[4 Lectures]**

Mass spectral fragmentation of organic compounds, common functional groups; molecular peak, McLafferty rearrangements, examples of mass spectral fragmentation of organic compounds with respect to their structure determination. **[4 Lectures]**

Laser spectroscopy and applications: Introduction to lasers, molecular beams. Optical pumping and double resonance. Quantum beats, photon echoes and free induction decay, applications in laser induced chemical reactions and coherent control, femtosecond chemistry and laser Raman spectroscopy. **[4 Lectures]**

[2 Lectures]

Photoelectron, Auger and X-ray fluorescence spectroscopy. Introduction and a few examples.

Text Book(s)

1. Banwell, C. N., Mc.Cash, E. M. *Fundamentals of Molecular Spectroscopy*, (Tata McGraw Hill, 1994).
2. Drago, R. S. *Physical Methods for Chemistry*, (Saunders Company, 1992).

Reference Book(s)

1. Nakamoto, K. *Infrared and Raman Spectra: Inorganic and Coordination Compounds, 6thedn.*, (John Wiley, 2009).
2. Pavia, D.L., G.M. Lampman, G.S. Kriz, J. R. Vyvyan, *Spectroscopy*, (Cengage India, 2008)

CH 714 Petrochemicals L 3 T 1 P 0 CR 4

Course Outcomes:

On completion of this course the students will be able to understand:

CO1: The primary raw materials for petrochemicals and their processing upto the value added product.
CO2: Crude oil processing and the production of hydrocarbon intermediates
CO3: Preparation and processing of synthetic petroleum based polymers

Course Contents:

Primary Raw Materials for Petrochemicals: Natural Gas, Crude Oils, Coal, Oil Shale, Tar Sand & Gas Hydrates [4 **Lectures]**

Hydrocarbon Intermediates: Paraffinic Hydrocarbons, Olefinic Hydrocarbons, Dienes, Aromatic Hydrocarbons, Liquid Petroleum Fractions & Residues **[4 Lectures]**

Crude Oil Processing and Production of Hydrocarbon Intermediates: [5 Lectures]

Physical Separation Process: Atmospheric Distillation, Vacuum Distillation, Absorption Process, Adsorption Process, Solvent Extraction

Conversion Processes: Thermal Conversion Processes, Catalytic Conversion Processes

Production of Olefins: Steam Cracking Hydrocarbons, Production of Diolefins

Chemicals based on Methane: Carbon Disulfide, Hydrogen Cyanide, Chloromethane, Ammonia, Methyl Alcohol, Oxo Aldehyde, Ethylene Glycol **[3 Lectures]**

Ethane and Higher Paraffins based Chemicals: Ethane Chemicals, Propane Chemicals, Isobutane Chemicals, Naphtha-based Chemicals, Chemicals from High-Molecular weight n-Paraffins **[3 Lectures]**

Chemicals based on Ethylene: Oxidation of Ethylene, Chlorination of ethylene, Hydration of Ethylene, Oligomerization of Ethylene **[4 Lectures]**

Chemicals based on Propylene: Oxidation of Propylene, Oxyacylation of Propylene, Chlorination of Propylene, Hydration of Propylene, Hydroformylation of Propylene, Disproportionation of Propylene **[4 Lectures]**

Chemicals based on Benzene, Toluene and Xylenes: Reaction & Chemicals of Benzene, Reaction & Chemicals of Toluene, Chemicals from Xylenes **[3 Lectures]**

Polymerization: Monomers, Polymers, Copolymers, Polymerization Reactions, Polymerization Techniques, Physical properties of Polymers **[3 Lectures]**

Synthetic Petroleum-based Polymers: Thermoplastics, Thermosetting Plastics, Synthetic Rubber, Synthetic Fibers [**3 Lectures]**

References:

1. Chemistry of Petrochemical Processes,2nd Edition, Sami Matar; Lewis F. Hatch, Gulf Publishing Company, United States of America,2000
2. Handbook of Petrochemicals and Processes. Margaret Wells, Ashgate Pub Co; 2 Sub edition (December 1999),ISBN-13: 978-0566080463

CH 715 Advanced Instrumental Methods in Chemistry

L 2 T 0 P 2 CR 4

Course Outcomes:

On completion of this course the students will be able to understand:

CO1: Use of different instrumental tools in the structure determination of chemicals and materials

CO2: Use of different instrumental tools in studying physico-chemical properties.

CO3: Use of instrumental tools in evaluating structure property evaluation

Course Contents:

Unit-1

Instrumentation, laboratory techniques and applications of UV-Visible, IR and Raman spectroscopy in physico-chemical studies and in structure determination of organic molecules and co-ordination compounds. **[6 Lectures]**

Unit-2 **[7 Lectures]**

Optical Rotatory Dispersion and Circular Dichroism: Deduction of absolute configuration, octane rule for ketones.

Unit-3 **[7 Lectures]**

Mass spectrometry: Instrumentation, mass spectral fragmentation of organic compounds, API and ESImode, LCMS, GCMS, applications to organometallic compounds, applications of FAB, MALDI experiment.

Unit-3 **[6 Lectures]**

NMR spectroscopy: Structural elucidation of molecules by NMR, Double resonance, saturation, Nuclear Overhouser effect (NOE) and dynamic nuclear magnetic resonance, ^{13}C NMR spectroscopy – chemical shift, ^{13}C coupling constant, 2D- NMR spectroscopy : NOISY, ROESY, HEPT, DEPT, INEPT terminology, Multinuclear NMR, Variable temperature experiments.

Unit-4 **[6 Lectures]**

EPR spectroscopy: Evaluation of g values and metal hyperfine coupling constants of metal ions, EPR spectroscopy of doublet radical systems.

Photoelectron spectroscopy: EXAFS, XPS, UPS spectroscopy, Neutron Powder Diffraction method.

Laser spectroscopy

Mössbauer Spectroscopy: Application to iron and tin compounds, detection of oxidation states and inequivalent MB atoms.

Unit-5 **[10 Lectures]**

Thermoanalytical methods: Thermogravimetric analysis, differential thermal analysis and differential scanning calorimetry.

Electrochemical methods: Coulometry, polarography, anode-stripping voltametry, pulse techniques, cyclic voltametry, electrogravimetry, spectroelectrochemistry.

Chromatographic methods: Adsorption, liquid-liquid partition, ion–exchange, paper and thin-layer chromatography, gel permeation chromatography and gas chromatography, size exclusion chromatography, HPLC, electrophoresis.

Radiochemical methods: Tracers in chemical analysis, isotopic exchange, isotopic dilution technique.

Unit-6 **[8 Lectures]**

Optical microscopy, transmission electron microscopy and scanning electron microscopy.
Atomic absorption spectroscopy, light scattering, neutron scattering, osmometry, tensiometry, ultrasonic absorption study.

Text Book(s)

3. Banwell, C. N., Mc.Cash, E. M. *Fundamentals of Molecular Spectroscopy*, (Tata McGraw Hill, 1994).
2. Hollas, J. M. *Modern Spectroscopy,* (John Wiley, 1996).

Reference Book (s)

1. Willard, H. H. *Instrumental Methods of Analysis*, (East West Press, 1998).
2. Nakamoto, K. *Infrared and Raman Spectra: Inorganic and Coordination Compounds, 6thedn.*, (John Wiley, 2009).

CH 716 Green Chemistry L 2 T 2 P 0 CR 4

Learning Outcomes:

On completion of this course the students will be able to understand:

CO1: Importance of green chemistry and its principle for sustainable environment
CO2: Designing a green synthetic protocol
CO3: Use of green reagents, green catalysts (zeolites, enzymes etc.) and green solvents
CO4: Environmental analytical chemistry

Course Contents:

Unit-1 **[16 Lectures]**

Introduction to the principals of green chemistry- prevention of waste, atom economy, less hazardous chemical syntheses;

Designing a green synthesis, clean routes, green reaction conditions- ultrasound assisted reactions, Microwave induced reactions, reaction in aqueous conditions, solid state and solid phase reactions.

Unit-2 **[20 Lectures]**

Green Processes: Substitute to water in various industries. Liquid CO_2.

CO_2 compatible surfactants for dry cleaning.

Use of green reagents, green catalysts (zeolites, enzymes etc.) and green solvents; applications of green chemistry (from laboratory to industries), Green chemistry in everyday life.

Environmental analytical chemistry, techniques and quantification of pollutants, trace element and radionuclide analysis.

Text Book(s)

1. Anastas, P. T. and Warner, J. C. *Green Chemistry: Theory and Practice*, (Oxford University Press, 1998).

Reference Book(s)

1. Cann, M. C. & Connelly, M. E. *Real World Cases in Green Chemistry,*ACS, , 2000.

CH 717 Computational Chemistry L 2 T 2 P 0 CR 4

Course Outcomes:

On completion of this course the students will be able to understand:

CO1: The basic hardware, software and operating system terminology and their significance
CO2: Different algorithms and programming
CO3: Numerical methods of scientific computing
CO4: Molecular mechanics calculation methods
CO5: The construction of z-matrix for some simples structures

Unit-1 **[18 Lectures]**

1. Introduction to basic hardware and software, bits, bytes, words, CPU, memory, operating systems (DOS, Windows, Unix).
2. Scientific computer uses, algorithm design, programming (with FORTRAN), error analysis
3. Numerical methods: Curve fitting, solution of polynomial equation, numerical integration, solution of ordinary differential equations, matrix multiplication, inversion and diagonalisation.
4. Basic principle of molecular mechanics, Monte Carlo, molecular dynamics, Extended Huckel Theory (EHT) and Hartree-Fock methods.
5. Isodesmic and homodesmotic equations.

Unit-2 **[18 Lectures]**

6. Exercise:
    i. Construction of Z-matrix for H_2CO
    ii. Construction of Z-matrix for H_2CO with molecular symmetry
    iii. Construction of Z-matrix using molecular symmetry for CH_3OH
    iv. Construction of Z-matrix using molecular symmetry for CH_4
    v. Construction of Z-matrix using a dummy atom for CO_2
    vi. Reading and interpreting output of GAMESS, dissociation energy of H_2O.
    vii. Examples for EHT including Walsh diagram for simple molecules

Text Book(s)

1. Lewars, E. *Computational Chemistry*, (Springer, 2003).
2. Balagurusamy, E. *Numerical Methods,* (Tata McGraw-Hill Publishing Company Limited, 2002

Reference Book(s)

1. Leach, A. R. *Molecular Modeling: Principles and Applications, 2nd edn.* (Pearson Prentice Hall, 2001).
2. Cramer, C. J. *Essentials of Computational Chemistry* (Wiley 2002).

CH 718 Nature and Applications of Surfactants L 2 T 0 P 2 CR 4

Course Outcomes:

On completion of this course the students will be able to understand:

CO1: Different aspects of interfacial phenomena

CO2: Characteristic features of surfactants and their structure-property relationship

CO3: Different applications of surfactants

Course Contents:

Unit-1 **[8 Lectures]**

Interfacial Properties: Adsorption of surfactants at interfaces, Gibbs adsorption isotherm, other adsorption isotherms (Langmuir, Frumkin, etc., surface and interfacial tension, ultra-low interfacial tension, interfacial rheology, wetting, foaming and dispersion by surfactant, flocculation by surfactant.

Unit-2 **[11 Lectures]**

Aggregation of surfactants and properties: Characteristic features of surfactants, hydrophobic interaction, cmc and factors affecting cmc, thermodynamics of micellization, micellar structure and shape, mixed micelles, Kraft point, cloud point, HLB, reverse micelle, biological membrane, solubilization.

Unit-3

Emulsification: Macroemulsion, miniemulsion, microemulsion, oil-water-surfactant phase diagram, de-emulsification, microstructure and properties of microemulsion, droplet size determination, partition of solutes in microemulsions.

Unit-4 **[4 Lectures]**

Speciality surfactants: polymeric surfactants, polymeric micelles, surfactant-polymer interaction, Liquid CO_2-compatible surfactants.

Unit-5 **[7 Lectures]**

Applications: Micellar catalysis, polymerization, petroleum processing and enhanced oil recovery, nanoparticle preparation, detergents, cosmetics and personal care, paints and pigments, paper and pulp technology, textile industry, mineral and ceramic processing, food technology, pharmaceuticals and agrochemicals, surfactants in green processes.

Unit-6 **[6 Lectures]**

Practical : Experiments on the above topics using the available laboratory facilities.

Text Book(s):

1. Rosen, M.J., *Surfactants and interfacial phenomena*, *4thedn.,* (John Wiley, New York, 2004).
2. Eastoe, J., *Surfactant science, 1stedn.,* (Wuhan University Press, Tai Yuan, China, 2004)

Reference Book(s)

1. Shah D.O., *Micelles, microemulsions and monolayers*, *1stedn*. (Marcel Dekker, New York, 1998).
2. Solans, C.; H. Kunieda, *Industrial applications of microemulsions*, *1stedn*.(Marcel Dekker, New York, 1997).

CH 719 Chemistry of Bioactive Molecules L 3 T 1 P 0 CR4

Course Outcomes:

On completion of this course the students will be able to understand:

CO1: Natural and synthetic bioactive molecules
CO2: Drug-receptor interactions
CO3: Isolation and retrosynthetic analysis of bioactive molecules
CO4: Spectroscopic applications to structure elucidation of bioactive molecules.

Course Contents:

Unit-1 **[25 Lectures]**

Interface of Chemistry and Biology, interaction between drug molecule and receptor sites, introduction to natural and synthetic bioactive molecules, detection and isolation of natural bioactive molecules, synthetic and semi-synthetic ways to different bioactive molecules, retrosynthetic analysis of simple bioactive molecules, art of synthesis, stereochemical consequences, synthetic strategies, tactics and protecting groups, modern spectroscopic applications to structure elucidation of bioactive molecules.

The development in the are in recent literature are also to be covered and this component is usually manipulated every year, e.g. total synthesis of taxol, AZT analogs, modified steroids etc.

Unit-2 **[11 Lectures]**

Group discussion and individual presentation on some recent hot topics in relevant chemistry.

Text Book(s)

1. Mann,. J; Davidson,R.S. ; . Hobbs, J.B; Banthrope , D.V. ; Harborne, J.B. *Natural Products, their chemistry and biological significance.* (Longmann, Essex, 1994).

2. Bohm H.J. ; Schneider, G. *Virtual Screening for Bioactive Molecules*, (Wiley-VCH, 2000).

Reference Book(s)

1. Nogradi, M. Stereoselective synthesis, A Practical approach, (VCH, Weinheim, 1995)

2. Greene , T. W. *Protecting groups in Organic synthesis*, (Wiley-VCH, 2000)

CH: 720: Density Functional Theory L 2 T 0 P 2 CR 4

Course Outcomes:

On completion of this course the students will be able to learn:

CO1: Fundamentals of Density functional theory

CO2: The use of DFT in the structure-property evaluation of some simple molecules.

Course Contents:

Unit-1 **[10 Lectures]**

1. Density matrices: Electron density, pair density, Fermi and Coulomb holes.
2. Thomas-Fermi model
3. Derivation of the Hohenberg-Kohn theorem
4. Kohn-Sham formalism
5. Different density functionals-LDA, GGA etc.

Unit-2 **[12 Lectures]**

6. Performance of DFT **[14 Lectures]**

i. Geometry optimization and vibrational frequencies of simple molecules.

ii. Charges on the atomic centers in a molecule, Mulliken population analysis, Reactivity descriptors.

iii. Van der Waals interaction, Lenard-Jones potential, counterpoise correction for Ar_2

iv. Molecules exhibiting Hydrogen bond, counterpoise correction for $(HF)_2$

v. Dissociation energies of $Ni(CO)_4$

Text Book(s) :

1. Koch, W. ; Holthausen, *M.C. A Chemist's Guide to Density Functional Theory, Second edn.,* (Wiley-VCH, 2001).

Reference Book(s)

1. Density-Functional Theory of Atoms and Molecules,Robert G. Parr and Weitao Yang, Oxford University Press, 1995.

CH 721 Dendritic Polymers L 3 T 1 P 0 CR 4

Course Outcomes:

On completion of this course the students will be able to learn:

CO1: Basic concepts of dendritic polymers

CO2: Synthetic methodology and characteristic properties of different types of dendritic polymers

Course Contents:

Unit-1 **[24 Lectures]**

Basic concepts of dendritic polymers: Introduction, historical background, significance, comparison with linear and star branched polymers, synthetic methodology : divergent, convergent, single step, accelerated approaches., characteristic properties ; applications ;

Unit-II **[12 Lectures]**

Brief review on different types of dendritic polymers : polyhydrocarbons, polyamides, polyalkinines, polyamidomines, polyethers, polyesters, silicon based dendritic polymers, phosphorous containing dendritic polymers, others.

Text Book(s)

1. Newkome, G.R (Ed.), *Advances in Dendritic Macromolecules, Vol. 1 – 5, (*CAI Press Inc. Greenwich, CT, 1994—99).
2. Newkome,G.R ; Moorefield. C.N. ; Vogtle,F. *Dendritic Molecules : Concepts, Synthesis, Prospectives, (*VCH, Weinhein, Germany, 1996).

Reference Book(s)

1. Frechhet J.M. J. ;Toamlia,D.A*Dendrimers and other Dendritic Polymers,*(John and Wiley & Sons, 2002).

CH 722 Polymeric Nanocomposites L 3 T 1 P 0 CR 4

Course Outcomes:

On completion of this course the students will be able to learn:

CO1: Fundamentals of polymer nanocomposites
CO2: Morphology and properties of polymer nanocomposite and their applications
CO3: Thermo-plastic and thermosetting polymer nanocomposites

Course Contents:

Unit-1 **[24 Lectures]**

Basic concept of polymer nanocomposites: Introduction, background, significance, structural characteristics of nanoparticles; preparative methods ; solution, in-situ polymerization, melt-

mixing, characterization : properties, morphology of polymer nanocomposite, mechanical, thermal, flame retardant, optical, electrical, electronic, applications ;

Unit-II **[12 Lectures]**

Brief description as a few thermo-plastic and thermosetting polymer nanocomposites.

Text Book(s)

1. Nicolais L. ; Cartenato G. (ed.), *Metal polymer nano composites*, (John & Wiley and Sons, Germany, 2004).

Reference Book(s)

1. Vaia R.A &Krishnamoorti J.R. (Ed.), *Polymer nanocomposites : synthesis, characterization and modeling* (ACS symposium series) (ACS, Oxford Press, Washington, 2001).

CH723 High Performance Polymers L 3 T 1 P 0 CR 4

Course Outcomes:

On completion of this course the students will be able to learn:

CO1: Structure and their characteristic properties of high performance polymer

CO2: Different types of High performance polymers

Course Contents:

Unit-1 **[16 Lectures]**

Introduction, structural characteristics, properties : thermal, electrical, optical, electronic ; applications,

Unit-II **[20 Lectures]**

Polymers: polyamides, polyimides, polycarbonates, polymers containing silicon, metal, fluorine, ladder and spiro polymers, liquid crystalline polymers.

Text Book(s)

1. Brydson, ,J.A . *Plastic Materials,(* Butterworth-Iteinemann, Oxford, 1999).

2. Turi E.A *Thermal characterization of polymeric materials (Vol. 1 & 2), (*Academic Press, California, 1997).

Reference Book(s)

1. Ghosh, M.K ; Mittal K.L (Ed.), *Polyimide fundamental and applications*, (Marcel Dekker, New York, 1996).

CH 724 Polymeric Biomaterials L 3 T 1 P 0 CR 4

Course Outcomes:

On completion of this course the students will be able to learn:

CO1: Basics of biocompatible polymers
CO2: Structure and properties of biopolymers
CO3: Synthetic Biopolymers

Course Contents:

Unit-1 **[13 Lectures]**

Introduction, biocompatibility of their requirements,

Unit-II **[23 Lectures]**

Structure and properties of natural biopolymers : proteins (silk, wool, hair etc.), polysaccharides, collagen, synthetic biopolymers : polylactic acid and its co-polymers, polyethylene oxides and it's copolymers, polyamidoamine, applications : medical, drug dealing etc.

Text Book(s)

1. Szycher,I.M. *High Performance Biomaterials,* (Technomic Publishing Co., Inc, Lancaster, 1991).
2. Goldberg , F.P ; Nakagima, A. *Biomedical Polymers*, (Academic Press, New York, 1980).

Reference Book(s)

1. Baker,R. *Controlled Release of Biomaterials*,(Academic Press, New York, 1980).
2. Dumitriu,S. *Polymeric Biomaterials(,* Marcel Dekker, Inc., New York, 1994)

CH 725 Catalytic Chemistry L 3 T 1 P 0 CR4

Course Outcomes:

On completion of this course the students will be able to understand:

CO1: Various aspects of homogeneous and heterogeneous catalysis
CO2: Different types of catalysis such as catalysis by enzyme, polymer, zeolites, solid surfaces, micelles etc.
CO3: Catalyst promotion and deactivation
CO4: Catalytic processes in petroleum industry

Course Contents:

Unit-1 **[12 Lectures]**

Catalysis in solution: Acid-base catalysis, catalysis by electron transfer, organometallic catalysis, catalysis by macromolecules, phase transfer catalysis, catalysis by micelles.

Catalysis by enzymes: Composition and structure of enzymes, reactions catalyzed by enzymes, nature of catalytic sites, supported enzymes.

Catalysis by polymers: Nature of polymers, catalysis by polymer gels, bifunctional and multifunctional catalysis, application of polymer catalysis.

Unit-2 **[12 Lectures]**

Catalysis by zeolites: Structure of zeolites, adsorption and diffusion in zeolites, catalytic cracking, other reaction of olefins, catalysis by zeolites containing metal complexes and clusters, nonzeolite molecular sieves, clays and other layered materials.

Catalysis on surface: Surface structures, catalysis on metal surfaces, catalysis on metal oxide surfaces, catalysis by supported metals.

Unit-3 **[12 Lectures]**

Reactors: Definition, classification, reactor design, choosing reactors in lab. and plant.

Catalyst promotion and deactivation: Promotion and promoters, causes and mechanism of deactivation, poisoning, sintering, prevention of catalyst decay, regeneration of catalysts Examples of heterogeneous catalytic reactions: Catalytic processes in petroleum industry-reforming, cracking and hydrotreating; hydrogenation, hydrodesulphurization, Fischer-Tropsch process, etc.

Text Book(s)

1. Bartholomew, C. H., Furrauto, R. J. *Fundamentals of Industrial Catalytic Processes 2nd edn.*, (Wiley Interscience, 2006).
2. Chakrabarty, D. K., Viswanathan, B. *Heterogeneous Catalysis* (New Age Int., 2008).

Reference Book(s)

1. Gates, B. C. *Catalytic Chemistry*, (John Wiley & Sons, 1992).
2. Augustine, R.L. *Heterogeneous Catalysts for Synthetic Chemists,* (Marcel- Dekker, 1996).

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