DEPARTMENT OF CHEMISTRY
NATIONAL INSTITUTE OF TECHNOLOGY
KURUKSHETRA

Master of Technology (M. Tech.) Program in

Molecular Engineering and Advanced Chemical Analysis

Sr. No	Course Code	Title	Total Credits			
			L	T	P	Credits
Semester I						
1	CHY-501T	Molecular Design and Synthesis	3	0	0	3
2	CHY-503T	Methods and Instrumental techniques for Chemical Analysis	3	0	0	3
3	CHY-505T	Advanced Materials-I	3	0	0	3
4*	CHY-507T, CHY-509T, CHY-511T, CHY-513T, CHY-515T, CHY-517T	Elective –I and II * Any two papers among these.	3	0	0	3
			3	0	0	3
5	CHY-519P	Computational Design and Chemical Synthesis Lab	0	0	4	2
6	CHY-521S	Seminar	0	0	1	1
			Total Credits			**18**
Semester II						
1	CHY-502T	Advanced Materials-II	3	0	0	3
2	CHY-504T	Advanced Spectroscopy and Separation Techniques	3	0	0	3
3*	CHY-506T, CHY-508T, CHY-510T, CHY-512T, CHY-514T, CHY-516T, CHY-518T, CHY-520T	Elective-I, II and III. * Any three papers among these	3	0	0	3
			3	0	0	3
			3	0	0	3
4	CHY-522P	Analytical Instrumentation Lab	0	0	4	2
5	CHY-524S	Seminar	0	0	1	1
			Total Credits			**18**
Semester III						
1	CHY-601P	Preparatory Work for Dissertation	0	0	20	10
			Total Credits			**10**
Semester IV						
1	CHY-602P	Dissertation	0	0	32	16
			Total Credits			**16**
Total Course Credits						**62**

List of Electives for Semester I*

Course Code	Title
CHY-507T	Chemistry of Nanomaterials and Characterization Techniques
CHY-509T	Solid State Chemistry
CHY-511T	Macromolecular Chemistry
CHY-513T	Conducting Polymers
CHY-515T	Environmental Chemistry
CHY-517T	Green Chemistry

***** Any two elective papers among these

List of Electives for Semester II*

Course Code	Title
CHY-506T	Sensor and Biosensor
CHY-508T	Molecular Catalysis
CHY-510T	Electro Analytical Chemistry
CHY-512T	Bio Chemistry
CHY-514T	Molecular Modeling and Computational Chemistry
CHY-516T	Cheminformatics
CHY-518T	Bioanalytical Chemistry
CHY-520T	Supramolecular Photo Chemistry and Sensor

*****Any three papers among these

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Molecular Design and Synthesis

Course Code: CHY-501T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I. Electronic structure methods for designing: Introduction to computational chemistry, Molecular modeling, Simulation and design, Fundamental concepts of molecular and quantum mechanics, Schrödinger equation, Born-Oppenheimer approximation, LCAO, self consistent field theory- MM, MD, DFT electron correlation method.

UNIT II. Method and Techniques in synthesis: Design of conventional and modern synthesis, Green synthesis, microwave synthesis, photochemical synthesis, Important reagents: Phase transfer catalysis (PTC), Dicyclohexylcarbodimide (DCC), Lithium diisoproyl amide (LDA) and selectivity.

UNIT III. Functional Molecules: Metalloporphyrin Fullerenes, Metalloenzymes, Composite materials, metallocene. Synthetic dyes, detergents, drugs, prodrugs, drug delivery, anti cancer agents (metal Complex)

UNIT IV. Molecular Electronics and Molecular machine: Logic gates, Molecular wires, Molecular switches, molecular shuttle, Molecular motors, Rotaxanes, catenanes. Liquid crystals, ionic liquid, dye-sensitized solar cell (DSSC).

Reference Books

1. Franck Jensen, Introduction to computational chemistry, 2nd Ed., John Wiley & Sons Ltd. (2007).
2. Advanced Organic Chemistry, Part A: Structure and Mechanisms, F. A. Carey and R. A. Sundberg, , Fifth edition, Springer, New York, 2007
3. Mechanism and theory in organic chemistry, Second edition, T. H. Lowry and K. S. Richardson, Harper & Row, New York, 198
4. Principle of Bioinorganic chemistry – Lippard and Berg, Univ. Science Books, 1994.
5. Principles of Fluorescence Spectroscopy, 3rd Ed., J. R. Lakowicz, Springer, New York, 2006.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Methods and Instrumental Techniques for Chemical Analysis

Course Code: CHY-503T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Basic principle, Instrumentation and application of following instruments: UV - Vis Spectrophotometry, Fluorescence Spectrometry, FT-IR and FT-Raman.

UNIT II: NMR techniques: 1D and 2D NMR techniques (Homo- and heteronuclear correlation (COSY, TOCSY, HSQC, HMBC)), ESI, Mass spectrometry.

UNIT III: Flame Emission, Atomic Absorption Spectrometry, XRD, Thermal analysis (TGA, DTA, DSC and ITC).

UNIT IV: Statistical methods in analytical chemistry (Uni-, Bi- and Multivariate data, Good Manufacturing Practices and related topics, complex examples).

Reference Books

1. Basic Principles of Spectroscopy Cheney R.Mac Grows Hill, 1971.
2. Thermal Method, Wendlandt, W.W. John, Wiley, 1986.
3. Principles of Instrumental analysis, Skoog, III rd edn., Sounders, 1985
4. D.W. Williams and Flemming, Spectroscopic methods of organic compound.
5. Banwell and McCash, Fundamentals of Molecular Spectroscopy, 4th Edition, Tata McGraw Hill, 2010.
6. Michael Hollas, Modern Spectroscopy, 4th Edition, Wiley, 2004
7. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 6th Edition, WileyInter Science, 2009.
8. William Kemp, Organic Spectroscopy, 3rd Edition, Macmillan, 2009

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Advanced Materials-I

Course Code: CHY-505T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: High energy material: Introduction, classification (explosives, propellants and pyrotechnics), historical overview, short introduction to detonation, density, deflagration, combustion, heat of formation, heat of detonation, stability and sensitivity, thermodynamics (detonation parameters, combustion parameters), new developments, Polymer Bonded Explosives (PBXs), secondary explosives and newly developed materials, new primary explosives, Oxidizers, experimental characterization of energetic materials (sensitivities, long-term stabilities, Gap test, etc.), special aspects of explosives (shaped charges, detonation velocities, Gurney model), significance of high nitrogen content, heterocycles, explosophoric groups, energetic salts, energetic co-crystals, molecular binding blocks, nitration reactions, energetic materials of the future.

UNIT II: Applications of Nanoparticle in various fundamental research, industries, medical field and environmental issue; toxicity, biosafety and ethical issue in application of Nanoparticle. Nano composite, organic materials, Energy applications of nanotechnology, Industrial applications of nanotechnology, Potential applications of carbon nanotubes.

UNIT III: Magnetic material: Introduction to magnetic materials, magnetic fields, magnetization and magnetic moment, magnetic measurements, magnetic materials, magnetic properties, magnetism in materials, magnetic domains, domain walls, domain processes, magnetic order and critical phenomena, electronic magnetic moments, quantum theory of magnetism, magnetics technological applications, soft magnetic materials, hard magnetic materials, magnetic recording, magnetic evaluation of materials.

Reference Books

1. P. W. Cooper, Explosive Engineering, Wiley-VCH, New York, 1997
2. J. Akhavan, The Chemistry of Explosives, RSC Paperbacks, Cambridge, 1998.
3. S. Fordham, High Explosives and Propellents, Pergamon, Press, Oxford, 1980.
4. R. Meyer, J. Kohler, A. Homburg, Explosives, Wiley-VCH, Weinheim, 2002.
5. Thomas M. Klapötke, Chemistry of High-energy Materials, Walter de Gruyter, 2011.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Elective Papers I-II

Master of Technology (M. Tech.) in Molecular Engineering and Advanced Chemical Analysis

Elective: Chemistry of Nanomaterials and Characterization Techniques

Course Code: CHY-507T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Nanochemistry Basics: Synthesis of nano structure top down and bottom up approach. Self assembly, Self assembling materials, Quantum Well, Quantum Dots, Super lattices & Layered Structures , two dimensional assemblies, Mesoscale self assembly, coercing colloids.
UNIT II: Chemical Patterning, Lithography & Nanocontact Printing: Soft lithography, Microlens arrays, Nonoring arrays, SAM crystal engineering, Sweet chips, Dip pen nanolithography, Nanoplotters, Nanoblotters.
UNIT III: Carbon nanostructures: C60, C70, carbon nanotubes (CNTs), clusters and their applications.
UNIT IV: Characterization: Powder X-Ray Diffraction, Electron Microscopies, Atomic force microscopy, Scanning tunneling microscopy, Small-Angle X-Ray Scattering, X-Ray Photoelectron Spectroscopy, Electronic Absorption Spectroscopy, Raman Spectroscopy.
UNIT V: Scope and opportunities: nanotechnology enabled sensors, microelectronics, and drug delivery.

Reference Books

1. Nanochemistry: A Chemical Approach to Nanomaterials, Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri, RSC Publishing
2. Nanochemistry, Kenneth J. Klabunde, Gleb B. Sergeev, Elsevier, 2013
3. Nanomaterials and Nanochemistry, C. Bréchignac, P. Houdy, M. Lahmani, Springer,
4. Concepts of Nanochemistry, Ludovico Cademartiri, Geoffrey A. Ozin, Wiley-VCH,
5. Nanoscale Materials in Chemistry, K. J. Klabunde, John Wiley & sons.
6. G. Ozin, A. Arsenault, Nanochemistry- A Chemical Approach to Nanomaterials. Springer. Wiley-VCH
7. Nanoparticles by G. Schmid , Wiley-VCH.
8. Nanoparticles-Building Blocks for Nanotechnology by V. Rottelo Kluwer Academic.
9. Nanoscale Materials by L. M. Liz-Marzan, P. V. Kamat, Kluwer Academic
10. Optical properties of metal clusters by Uwe kreibig and Michael Vollmer.
11. T. Pradeep, Nano: The essentials, McGraw-Hill Education, New Delhi.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Solid State Chemistry

Course Code: CHY-509T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Electronic structure of solids: Introduction, Simple non-metallic solids, Transition metal compounds, Defects and impurities.

UNIT II: Superconducting Materials : Introduction, zero resistance phenomenon, Meisner effect, Critical temperature, Qualitative features of microscopic theory of superconductivity, Basics ideas of BCS theory, Superconductivity and magnetism.

UNIT III: Zeolite: Introduction, Structures, compositions, Geological occurrence, Zeolite synthesis, Aluminomsilicate gel, Crystalline mechanisms, Zeolites as ion exchangers, Zeolite catalysts, Metal complex incorporated zeolites and catalytic applications, Interconversion of aromatics by Zeolites, Clays, pillared clays, and layered double hydroxides, Hydroxy appetites.

UNIT IV: Ferroics: Introduction, Proper and Improper ferroics, Primary and secondary Ferroics, Ferroelectrics, Relaxor ferroics.

Reference Books

1. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 1984.
2. L. Smart and E. Moore, Solid State Chemistry - An Introduction, Chapman & Hall, 1992.
3. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, 1993.
4. K. Chakrabarty, Solid State Chemistry, New Age Publishers, 1996.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Macromolecular Chemistry

Course Code: CHY-511T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Basic Concepts: Monomers, repeat units, functionality, degree of polymerization, types of polymerizations, different types of polymerization process, polymerization in homogeneous and heterogeneous systems and importance of polymers.

UNIT II: Structure and Properties: Morphology and order in crystalline polymers - configurations of polymer chains, crystal structures of polymers, morphology of crystalline polymers, strain – induced morphology, crystallization and melting, polymer structure-property relationship and polymer degradation.

UNIT III: Polymer Processing: Introduction to plastics, elastomers and fibers. Constituents of plastics – binders, fillers, dyes and pigments, plasticizers, lubricants and catalysts. Fabrication of plastic articles – casting, blowing, extrusion, lamination and moulding: cold moulding, compression moulding, injection moulding and transfer moulding.

UNIT IV: Properties of Commercial Polymers: Polyethylene, Polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers - Fire retarding polymers and electrically conducting polymers. Biomedical polymers - contact lens, dental polymers, artificial heart, kidneys, skin and blood cells.

Reference Books

1. Physical Chemistry of Macromolecules: Basic Principles and Issues by S. F. Sun, 2nd Edition, 2004
2. Macromolecular Chemistry, Volume 1, A D Jenkins, John F Kennedy, Royal Society of Chemistry, 1980.
3. V. R Gowarikar, Vishwanathan Srikanth, Polymer Chemistry, Wiley Estern, Bombay, 2000.

Note: The paper setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Conducting Polymers

Course Code: CHY-513T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Introduction and classification of CP: Introduction, redox polymers, intrinsically conducting polymers, electronically conducting polymers with pendant redox functionalities, copolymers, composite polymers, Chemical and electrochemical synthesis of conducting polymers

UNIT II: Methods of investigation: electrochemical methods (cyclic voltametry, chronamperometry and chronocoulometry, electrochemical impedance spectroscopy), in situ combination of electrochemistry (electrochemical quartz crystal nanobalance, radiotracer techniques, probe beam deflection technique, ellipsometry, spectroelectrochemistry, scanning probe techniques, conductivity measurements), other techniques (scanning electron microscopy, X-ray photoelectron spectroscopy, X-ray diffraction and absorption).

UNIT III: Redox transformations and transport processes: electron transport, ion transport, coupling of electron and ionic charge transport, solvent transport, effect of film structure and morphology, relaxation and hysteresis phenomena, measurement of rate of charge transport.

UNIT IV: Applications of conducting polymers: material properties of conducting polymers, applications in various fields: thin film deposition and microstructuring of conducting materials, electroluminescent and electrochromic devices, membranes and ion exchange, corrosion protection, sensors, materials for energy technologies, artificial muscles, electrocatalysis.

Reference Books

1. A. Ravve, Principles of Polymer Chemistry, Plenum Press, New York, 2000
2. Charles Tanford, Physical chemistry of macromolecules , John Wiley & Son.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Environmental Chemistry

Course Code: CHY-515T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Introduction, Chemistry and understanding our environment (pollution, pollutant, its effects and causes), human population growth and environment, sustainability and carrying, pollution-classification and effects, environmental perspectives, environmental hazards or disasters.

UNIT II: Biogeochemical cycles in environment: introduction, sulphur cycle, phosphorus cycle, carbon hydrogen cycle, oxygen cycle, nitrogen cycle, biological control of environmental factors, production and decomposition in nature, biodistribution of elements

UNIT III: Greenhouse effect and global warming: green house effect, green house gases and sources, climate change, global warming and facts, global warming and walker circulation, global warming and fossil fuels, global warming and domino effect, global warming and forests, forest fires, global warming and water cycle, global warming and acid rain, global warming and carbon cycle, global warming and galcier, control and remedial measures, technologies to arrest global warming, latest about global warming.

UNIT IV: Environment friendly technologies: introduction, eco-technology, organic farming and advances, Integrated plant nutrient and pest management, soil solarisation, watershed and water management.

Reference Books

1. Environment Chemistry by A. K. de
2. Environmental Chemistry by M. Satake, S. Sethi and S.A. Eqbal.
3. Environmental and Man Edited by J. Lenihan and W.W. Fletcher

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Green Chemistry

Course Code: CHY-517T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Principles and concepts of green chemistry (Introduction, sustainable development-green engineering, atom economy, atom economic reactions, atom un-economic reactions, reducing toxicity)

UNIT II: Waste: production, problems and prevention, problems caused by waste, sources of waste form industry, waste minimization techniques, on-site treatment: physical, chemical and biotreatment; design for degradation, polymer recycling)

UNIT III: Measuring and controlling environmental performance (importance of measurement, life cycle assessment, green process metrics, and environmental management system).

UNIT IV: Catalysis and Environmentally benign organic solutions: introduction, heterogeneous catalysis, homogeneous catalysis, phase transfer catalysis, biocatalysis, photocatalysis; organic solvents and volatile organic solvents, solvent free systems, supercritical fluids, water as reaction solvent, ionic liquids, fluorous biphase solvent, comparing greenness of solvents.

UNIT V. Renewable sources and greener technologies: biomass as renewable source, energy from - biomass, fossil fuels, solar power, fuel cells, other form of renewable sources, alternative economics, hydrogen economy and syngas economy, biorefinery; photochemical reactions, chemistry using microwaves, sonochemistry, electrochemical synthesis, approach to green chemical industry, designing of greener processes, industrial case studies, future of green chemistry.

Reference Books

1. V. K. Ahluwalia, M. Kidwai, New trends in Green Chemistry, New Age Publications, 2004.
2. P.T. Anastas and J.C. Warner, Green Chemistry, Theory and Practice, Oxford University Press, 2000.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Computational Design and Chemical Synthesis Lab

Course Code: CHY-519P

L T P C
0 0 4 2

Sessional -50 Theory 50
Duration of Exam-3 hrs

1. Determination of rate constant of reaction: oxidation of iodide ion by bromate solution.

2. Multistep synthesis of organic molecules (i) acridone from anthranilic acid (ii) N-phenylanthranilic acid from o-toludine (iii) sym-tribromobenzene from nitrobenzene (iv) p-aminophenol from benzene and their characterizations by CHN, IR, NMR, TGA and GC mass analysis.

3. Multi-dimensional NMR studies of biomolecules.

4. Analysis of environmental samples by Gas-Chromatography.

5. Optimization and molecular engineering of small organic molecules by computational methods.

6. (a) Synthesis and characterization of transition and inner-transition metal coordination compounds.
   (b) Synthesis of transition metal-Schiff base complex and their biological activity (anti-fungal, Gel-electrophoresis).

7. Preparation of simple organometallic compounds.

8. Chemiluminescence property of Eu/Tb based inorganic materials (life time measurement).
9. Single crystal growth by various techniques.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Seminar

Course Code: CHY-521

L T P C
0 0 1 1

Sessional -50 Theory 50
Duration of Exam-1 hrs

Semester II

Master of Technology (M. Tech.) in Molecular Engineering and Advanced Chemical Analysis

Advanced Materials-II

Course Code: CHY-502T

L T P C
0 0 4 2

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Biomaterials: Introduction to biomaterials, performance of biomaterials, historical background, metallic biomaterials, ceramic biomaterials, polymeric and biodegradable biomaterials, composite biomaterials, biofuctional hydrogels, soft tissue replacement, hard tissue replacement, biomechanics, biomaterial interactions, wound healing biology, cellular mechanics, materials-host interactions, biomaterials testing, statistics, regulatory considerations, intellectual property, standardized materials testing.

UNIT II: Photovoltaic material; Photovoltaic materials and phenomena, applications, types of semiconductor junctions, crystalline silicon, amorphous silicon, gallium arsenide and other III-V materials, cadmium telluride and other II-VI materials, copper indium diselenide and other I-III-VI materials, materials interested for solar cells. Dye sensitized solar cells.

UNIT III: Gas capture and storage; MOF in Gas capture and storage.

Reference Books:

1. Solar Photovoltaics: Fundamentals Technologies and Applications, Solanki PHI Learning Pvt. Ltd., 2009.
2. Cheetham, A.K. *Solid state chemistry: compounds*; Oxford University Press: Oxford, 1992 (ISBN: 0198551665, 9780198551669).
3. Lalena, J.N.; Cleary, D.A. *Principles of Inorganic Materials Design* ; Wiley: New York, 2010 (ISBN: 978-0-470-40403-4)

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Advanced Spectroscopy and Separation Techniques

Course Code: CHY-504T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: XRF, Polarography, cyclic voltametry, Microscopy and Imaging (optical fluorescence, SEM, AFM, TEM), Electron Spectroscopy for Chemical Analysis (ESCA), ICPE, Circular dichroism (CD), optical rotary dispersion.

UNIT II: Separation techniques: Introduction, General principle, Basic concepts of separation, Separation based on phase equilibria, Separation based on rate phenomena (barrier separations, field separations), Decantation, Filtration, Centrifugation, Evaporation, Crystallization, Distillation, Fractional distillation, Sublimation, Chromatography (HPLC and GC).

UNIT III: Modern separation techniques in Organic chemistry, Phase labeling, Polymer based separation and purification techniques, advantages and disadvantages of these methods.

Reference Books:

1. Solvent extraction in analytical A chemistry by G.H. Morrison, F. Frieiser, John Wiley & Sons, NY.
2. Ion exchange and solvent extraction of metal compounds by Y. Macros, A.S.Kertes,
3. Wiley, Interscience.
4. O. Samuelson, Ion exchange separation in Analytical Chemistry, J.Wiley & Sons.
5. A. I. Vogel, A Text Book of quantitative Inorganic Analysis, Longmann Green.
6. D.A. Skoog & D.M. West, Fundamentals of Analytical Chemistry - Holy Rinchart.
7. G.W. Ewing, Instrumentation Methods of Chemical Analysis, McGraw Hills.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Elective Papers III-V

Master of Technology (M. Tech.) in Molecular Engineering and Advanced Chemical Analysis

Elective: Sensor and Biosensor

Course Code: CHY-506T

L T P C
3 0 0 3

Sessional-50 Theory 50
Duration of Exam-3 hrs

UNIT I: Sensors and transducers: An overview, electrochemical sensors, Semiconductor devices as chemical sensors, Optical chemical sensors, Piezoelectric sensors, Sensor signal processing.

UNIT II: Biosensors: Chemistry of biomolecules and their immobilization for biosensors, Types of biosensors and their application - Environmental monitoring, process control, and clinical/biochemical analysis,

UNIT III: Amperometric biosensors, Immunosensors based on Surface Plasmon Resonance techniques, Principle and fabrication of DNA arrays, Trend of biosensor development, Electronics in sensing, Lab on chip.

Reference Books:

1. Sadana and N. Sadana, Handbook of Biosensors and Biosensor Kinetics, Amsterdam; London: Elsevier Science, 2010.
2. U. E. Spichiger-Keller, Chemical Sensors and Biosensors for Medical and Biological Applications, Weinheim; New York: Wiley-VCH, 1998.
3. J.-M. Lehn; Supramolecular Chemistry-Concepts and Perspectives (Wiley-VCH, 1995)
4. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press, 1999)
5. J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000)

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Molecular Catalysis

Course Code: CHY-508T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I : Homogeneous catalysis: Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions. Acid-base catalysis, general acid base catalysis, mechanism of acid –base catalysis, catalytic activity and acid-base strength- Bronsted relationships.

UNIT II: Heterogeneous catalysis: Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials. Preparation of metal catalysts , supported metal catalysts and non- metallic catalysts.

UNIT III: Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts- Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Catalytic activity – the determining factors.

UNIT IV: Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants for oxidation and reduction of organic compounds.

Reference Books:

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker and A. V. Ramaswamy, Narosa Publishing House.
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry, M. Satake, Y. Hayashi, Y.Mido, S. A. Iqbal and M. S. sethi.
6. Physical Organic Chemistry by L.P.Hammett, unit 9, Mc Graw Hill.
7. Chemical Review, 57, 1935(1957), M.A. Paul and F.A. Long.

8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press.
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim.
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer.
11. Hand book of phase transfer catalysis Edited by Y. Sasson and R. Neumann.
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler and E. J. Feudler, Academic Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed), Plenum.
14. Micelles – Theoretical and Applied aspets, V.Moroi, plenum.
15. Physical Chemistry of surfaces, A.W.Adamson and A.P. Gast, Wiley
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic chemistry.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Electro Analytical Chemistry

Course Code: CHY-510T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT-I: Basic Principles of Electrochemistry and Review of fundamental concepts.

UNIT-II: Potentiometry: Reference Electrodes, Ion-Selective Electrodes, Direct Potentiometric Measurements, Potentiometric Titrations and Application.

UNIT-III: Coulometry and Electrogravimetry: Electrogravimetry, Controlled-Potential Coulometry, Constant-Current Coulometric Titrations.

UNIT-IV: Modern Voltammetric Techniques: Pulse Voltammetry, Fast Linear Sweep Voltammetry, Anodic Stripping Voltammetry and Amperometric Titrations.

Reference Books:

1. A. J. Bard and L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd Edition., New York: Wiley, 2001.
2. J. Wang, Analytical Electrochemistry, 2nd Edition, Wiley, 2000.
3. R. Greef, R. Peat, L.M. Peter, D. Pletcher and J. Robinson, Instrumental Methods in Electrochemistry, Ellis Horwood, 1990.
4. P.T. Kissinger and W.R. Heineman, editors, Laboratory Techniques in Electroanalytical Chemistry, 2nd Edition, Marcel Dekker, 1996.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Bio Chemistry

Course Code: CHY-512T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT-I: Nucleic Acids: Watson - Crick Model of DNA structure. A, B and Z - DNA Cruciform structure in DNA, secondary and tertiary structure of RNA, methods for nucleic acid sequence determination, isolation and purification of DNA, mRNA, rRNA and tRNA.

UNIT-II: Vitamins and Porphyrine: Vitamins - water soluble - thiamine, riboflavin, niacin, pyridoxine, folic acid, ascorbic acid- sources, structure, biochemical functions, deficiency diseases, daily requirements; fat soluble - vitamin A, vitamin D2, vitamin E and vitamin K - sources, structure, biochemical functions, deficiency diseases, daily requirements. Porphyrin ring system, chlorophyll, hemoglobin, myoglobin and cytochrome.

UNIT-III: Proteins and Electrophoresis: Isolation, fractionation and purification of proteins. Denaturation and renaturation of proteins. The peptide bond: Ramachandran plot. Electrophoresis: General principles. Electrophoresis of nucleic acids - agarose gel electrophoresis, DNA sequencing gels, pulsed field gel electrophoresis.

UNIT-IV: Enzymology: Enzymes classification active site identification and Conformation. Michaelis-Menten Kinetics of monosubstrate enzyme reaction, Allosteric Enzymes-Kinetics Significance of Sigmoidal Behaviour, Role in Metabolic Regulation.

Reference Books:

1. Biochemistry by L. Stryer, W.H. Freeman and Co. 5th 2002
2. Fundamentals of Biochemistry by Voet and Voet, John Wiley and sons NY (2002).
3. Lehninger's Principle of Biochemistry by David L. Nelson and Michael M. Cox. W. H. Freeman; 4th edition (2004)
4. Text Book of Biochemistry with clinical correlation by Thomas .M. Devlin, John Wiley-Liss, Hobokhen NJ publishers (2006)
5. Biochemistry by Zubey, GL WCB Publishers.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Molecular Modeling and Computational Chemistry

Course Code: CHY-514T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT-I: Molecular Modeling: Introduction to molecular modeling: Energy minimization, geometry optimization, conformational analysis, global conformational minima determination; Approaches and problems; Bioactive vs. global minimum conformations; Automated methods of conformational search; Advantages and limitations of available software; Molecular graphics; Computer methodologies behind molecular modelling including artificial intelligence methods.

UNIT-II: Hartee Fock Methods, Post- Hartee Fock Methods and Basis sets: Semi empirical methods. Perturbation theory, Coupled cluster theory, Configuration interaction. Density functional theory. Basis sets- Stater type and Gaussian type basis functions, classification of basis sets-minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets. Correlation consistent basis sets.

UNIT-III: Computing thermodynamics and Molecular properties: Input of molecular structure- Z matrix construction. Single point energy calculations. Optimizations-analysis of Gaussian output files. Computation of UV-visible, fluorescence, IR and NMR spectra. Transition barrier and activation energy, potential energy surface.

UNIT-IV: Introduction to Bioinformatics: Definition and History of Bioinformatics, Introduction to Data Mining, Applications of Data Mining to Bioinformatics problems and Applications of Bioinformatics.

Reference Books:

1. I. N. Levine, Quantum Chemistry, 6th edition, Pearson Education Inc., 2009.
2. Foresman and A. Frish, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
3. C. J. Cramer, Essentials of Computational Chemistry: Theories and models, John Wiley & Sons, 2002.
4. Jan H. Jensen, Molecular modelling basics, CRC press, Taylor & Francis Group, 2010.
5. P. W. Atkins & R. S. Friedman, Molecular quantum mechanics, 4th edition, Oxford university press, 2005.

6. F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 1999.
7. David C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001Errol G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd edition, Springer, 2011.
8. Introduction to Bioinformatics: A Theoretical and Practical Approach by Stephen A. Krawetz. Oxford University Press.
9. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Cheminformatics

Course Code: CHY-516T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Introduction to Cheminformatics: Introduction to cheminformatics, History and Evolution of cheminformatics, Use of cheminformatics, Prospects of cheminformatics, Molecular Modeling and Structure Elucidation.

UNIT II: Representation of Molecules and Chemical Reactions: Nomenclature; Different types of Notations; SMILES coding; Matrix Representations; Structure of Molfiles and Sdfiles; Libraries and toolkits; Different electronic effects; Reaction classification.

UNIT III: Searching Chemical Structure: Full structure search; sub structure search; basic ideas; similarity search; Three dimensional search methods; Basics of Computation of Physical and Chemical Data and structure descriptors; Data visualization.

UNIT IV: Computer Assisted Virtual screening design: Structure Based Virtual Screening- Protein Ligand Docking, Scoring Functions for Protein Ligand docking, Practical aspects of structure based Virtual Screening; Prediction of ADMET Properties, 2 D and 3D data searching, Chemical databases, Role of computers in Chemical Research.

UNIT V: Application of Cheminformatics in Drug Design: Quantitative Structure-Property Relations; Descriptor Analysis; Computer Assisted Structure elucidations; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design.

Reference Books:

1 Andrew R. Leach, Valerie J. Gillet, Cluwer , Introduction to Cheminformatics, Academic Publisher, Netherlands, 2003.
2. Lisa B. English (Editor), Combinatorial Library Methods and Protocols, Humana Press Inc, Volume: 201, 2002.
3. Frank Jensen, Introduction to Computational Chemistry, Wiley Publisher, Second Edition, 2006.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Bioanalytical Chemistry

Course Code: CHY-518T

L T P C
3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Body fluids: Composition and detection of abnormal level of certain constituents leading to diagnosis, sample collection and preservation of physiological fluids, analytical methods for the constituents of physiological fluids (blood, urine).

UNIT II: Blood, Urine and Enzymes: Blood-Estimation of glucose, cholesterol, urea, haemeglobin and bilirubin. Urine- Urea, uric acid, creatinine, calciumphosphate, sodium, potassium and chloride. Enzymes- Biological significance, analysis and assay of enzymes (pepsin, tyrasinase), vitamins (thiamine ascorbic acid, vitamin A) and harmones (progesterone, oxytocin, insulin), chemical, instrumental and biological assays to be discussed wherever necessary.

UNIT III: Forensic analysis: General discussion of poisons with special reference to mode of action of cyanide organophosphates and snake venom, estimation of poisonous materials such as lead, mercury, and arsenic in biological materials.

UNIT IV: Food Analysis: Historical perspectives, objectives of food analysis. Oils and fats and their analysis-iodine value, saponification value and acid value. Rancidity-detection and determination (peroxide number). Tests for common edible oils. General methods for the determination of moisture, crude fibre and ash contents of foods. Analysis of milk for fat and added water. Determination of chicory and caffeine in coffee;caffeine and tannin in tea. Coloring matters in foods classification, certified colours, detection of water soluble dyes, colour in citrus fruits, beet dye in tomato products, mineral colour. Pesticide residues in foods. Determination of chlorinated organic pesticides.

Reference Books:

1. Pharmaceutical Analysis, T. Higuchi and E.B. Hanssen, John Wiley and Sons, NewYork.
2. Quantitative Analysis of drugs, P.D. Sethi, 3rd edition, CBS Publishers, New Delhi, 1997.
3. Practical Clinical biochemistry methods and interpretations, R. Chawla, J. P. Bothers Medical Publishers (P) ltd., 1995.
4. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.

5. Pharmaceutical Analysis, Modern methods-Part A and B, Edited by James W. Munson.
6. The Essentials of Forensic Medicine and Toxicology-Dr.K.S. Narayana Reddy.
7. Practical clinical Biochemistry-Harold Varley and Arnold.Hein mann, 4th edn.
8. Analysis of Foods-H.E.Cox.
9. Chemical Analysis of Foods-H.E.Cox and pearson.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Elective: Supramolecular Photo Chemistry and Sensor

Course Code: CHY-520T

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3 0 0 3

Sessional -50 Theory 50
Duration of Exam-3 hrs

UNIT I: Principles and concepts: Jablonski diagram and photophysical processes, Franck-Condon principle. Excited state lifetime, steady state and time resolved emission, factors affecting excited state energy: solvent effect, TICT. Quantum yield expressions, excimer and exciplex, kinetics of luminescence quenching: static and dynamic, Stern-Volmer analysis, deviation from Stern-Volmer kinetics.

UNIT II: Photoinduced electron transfer rates, free energy dependence of electron transfer on rate, Photoinduced energy transfer, FRET, rate and efficiency calculation of FRET. Methods: Measurement of fluorescence and phosphorescence and lifetimes.

UNIT III: Applications: Fluorescence based sensors – examples of molecular and supramolecular systems. Crown ethers, cryptands, spherands, cyclodextrins and calixaranes Anion sensor, Cation sensor, Bio-sensor, and optimization of supramolecular receptor.

Reference Books:

1. Fundamentals of Photochemistry, K. K. Rohatgi-Mukherjee, New Age International, 1978.
2. Organic Photochemistry and Photophysics (Molecular and Supramolecular Photochemistry), CRC Press, V. Ramamurthy (Editor).
3. Fluorescence Sensors and Biosensors , CRC Press, Richard B. Thompson.
4. Fundamentals of Photoinduced Electron Transfer, G. J. Kavarnos, VCH publishers Inc., New York, 1993.
5. Molecular Fluorescence: Principles and Applications, B. Valeur, Wiley-VCH Verlag GmbH, Weinheim, 2002.

Note: The Paper Setter is requested to set eight questions in all. The students are required to attempt any five questions.

Master of Technology (M. Tech.) in
Molecular Engineering and Advanced Chemical Analysis

Analytical Instrumentation Lab

Course Code: CHY-522P

L T P C
0 0 4 2

Sessional -50 Theory 50
Duration of Exam-3 hrs

1. Spectrophotometric estimations of (i) Fe^{III} as thiocyanate complex (ii) phosphate as phosphomolybdate (iii) Fe^{II} and Fe^{III} mixture as 1,10 phenanthroline complex.
2. Spectrophotometric identification and determination of biomolecules (carbohydrate, amino acids, proteins and cholesterol) by UV-Vis and IR spectroscopy.
3. Determination of composition of various mixtures spectrophotometrically (i) crystal violet and aurine (ii) Potassium dichromate and potassium permanganate.
4. Separation of organic molecules by chromatographic techniques (CC, TLC, HPLC).
5. Synthesis, characterization and prediction of energetic properties of materials through theoretical and experimental (DSC) studies.
6. Simple biochemical preparations starting from natural sources (i) Lactose and casein from milk (ii) Mucic acid from milk (iii) Lycopene from tomato.
7. Synthesis, characterization and properties study of oxide/ doped metal oxide nanoparticles by TGA-DTA, DSC, ITC, IR, UV-Vis, PL, PXRD, SEM and TEM.
8. Synthesis of conducting polymers. Studies of their ionic conductivity and optical properties.
9. Electronic and magnetic properties of complex metal oxides.

Master of Technology (M. Tech.) in Molecular Engineering and Advanced Chemical Analysis

Seminar

Course Code: CHY-524S

L T P C
0 0 1 1

Sessional -50 Theory 50
Duration of Exam-1 hrs

Semester III

Master of Technology (M. Tech.) in Molecular Engineering and Advanced Chemical Analysis

Course Code: CHY-601P

L T P C
0 0 20 10

Preparatory Work for Dissertation

Semester IV

Master of Technology (M. Tech.) in Molecular Engineering and Advanced Chemical Analysis

Course Code: CHY-602P

L T P C
0 0 32 16

Dissertation