DEPARTMENT OF APPLIED CHEMISTRY

M.Phil Course Structure (2018 Regulation)

Course	Subject	Credits	Marks		
			Continuous Evaluation	End Semester Examination	Total
I SEMESTER					
CHE 4101	Research Methodology	4	50	50	100
CHE 4102	Literature Review	2		100	100
CHE 4103	Modern Methods in Chemistry	4	50	50	100
CHE 4104 A - CHE 4104 O	Elective Course CHE 4104 A to CHE 4104 O	4	50	50	100
II SEMESTER					
CHE 4201	Project Evaluation	8	100	100*	200
	Viva-voce	4	-	100	100
Total Credit		**26**	**250**	**450**	**700**

Elective courses for M.Phil

1.	Chemical Instrumentation	CHE 4104	A
2.	Inorganic Chemistry	CHE 4104	B
3.	Quantum Chemistry	CHE 4104	C
4.	Organic Chemistry – Terpenoids	CHE 4104	D
5.	Organic Chemistry – Lipids	CHE 4104	E
6.	Organic Synthesis	CHE 4104	F
7.	Organic Chemistry (Heterocyclic compounds and natural products having heterocyclic systems)	CHE 4104	G
8.	Physical Chemistry – (Electrochemical Methods)	CHE 4104	H
9.	Adsorption and Catalysis	CHE 4104	I
10.	Chemistry of Polymers	CHE 4104	J
11.	Pericyclic Reactions and Photochemistry	CHE 4104	K
12.	Polymer Composite	CHE 4104	L
13.	Enzyme Technology	CHE 4104	M
14.	Advanced Computational Chemistry	CHE 4104	N
15.	Chemistry of Nanomaterials	CHE 4104	O

CORE

CHE 4101 - Research Methodology and Quantitative Techniques

(4 credit) **64 hours**

UNIT 1

Research methodology – Defining the research problem – Literature Survey and obtaining Scientific Information using Library and Online resources – primary, secondary and tertiary literature, including the major abstract journals, data sources, compendia, patents, current awareness, and computer readable sources – Introduction to GLP – Laboratory Safety – Green chemistry.

UNIT 2

Statistics for chemists – Errors – Describing Data – Frequency distributions – Hypothesis tests – Comparison of means – t-test – F- test - Q-test - Confidence in linear regression – Sequential Data – correlograms – Linear smoothing functions and filters – Fourier transforms – peak shapes in spectroscopy and chromatography - Application of spread sheets in Data Analysis.

UNIT 3

Experimental Design – Degrees of freedom and sources of error – Analysis of variance and interpretation of errors – Randomization and blocking – Two way ANOVA – Latin Squares and other designs – Interactions - Matrices, vectors and pseudo inverse – Design Matrices – Factorial Designs – Fractional factorial Designs.

– Mixtures – simplex optimizations – Introduction to multivariate analysis – Neural networks – Computer applications in experimental design.

UNIT 4

Computational Chemistry - Open source Computational chemistry softwares - Potential Energy Surfaces, Molecular Mechanics - Introduction to Molecular Orbitals. Semi-empirical MO Methods, One Electron Properties - Basis sets, Geometry Optimization - Calculating Vibrational Frequencies - Transition States and Reaction Paths - Electron Correlation, Density Functional Theory - SCF Convergence - Solvation - Excited States - MM/QM calculations -

UNIT 5

Communication of scientific information – Scientific paper – communications – Notes– Reviews – Scientific talk – Poster presentation – Research proposals – Presenting data in tables and figures – Criticisms and evaluation of Scientific Research.

Suggested Reading

1. Ivan Valiela, Doing science: Design, analysis and Communication of Scientific Research; Oxford University Press, 2001.
2. C. R. Kothari, Research Methodology, Methods and Techniques; New Age International Publishers. 1990.
3. R. G. Brereton, Applied Chemometrics for Scientists; John Wiley and Sons Ltd. 2007.
4. D. L. Massart, B. G. M. Vandeginste, S. M. Deming, Y. Michotte, L. Kaufman, Chemometics: A Text Book; Elsevier, 2003.
5. J. N. Miller, J. C. Miller, Statistics and Chemometrics for Analytical Chemistry; Person Prentice – Hall, 2005.
6. P. Laszlo, Communicating Science: A Practical Guide; Springer, 2006.
7. A. R. Leach, Molecular Modelling: Principles and Applications; 2nd ed., Prentice Hall, 2001.

CORE

CHE 4103 – Modern Methods in Chemistry

(4 credit) **64 hours**

UNIT 1- Advanced Quantum Chemistry and Chemical Bonding

Chemical bonding, Born Oppenheimer approximation, The variation method, LCAO-MO method, Huckel MO theory. Molecular orbital method for diatomic molecules, Correlation diagram, Non-crossing rule. Valence bond method. Comparison of VB and MO method, Bonding in simple molecules like water, BF_3, NH_3 CH_4. VSEPR theory, Pi bonding in simple molecules. HMO method for linear conjugated hydrocarbons, aromatic hydrocarbons. Ethylene, Allyl and Cyclopropenyl systems, butadiene, cyclobutadiene and benzene. Calculation of free valence charge density and reactivity.

Wave functions as basis for irreducible representations, symmetry adapted linear combinations. Construction of hybrid orbitals for AB_3(planar), AB_4(Td), AB_5(D3h) and AB_6(Oh) type of molecules Use of symmetry in HMO using Naphthalene as an example.

Symmetry-based selection rules for cyclization reactions. MOS for regular octahedral and tetrahedral, molecules. MOS for Ferrocene.

UNIT 2 Computational Chemistry

Tools and philosophy of computational chemistry. Fundamental molecular forces-the dynamic equation. Separation of variables. Separation of variables and hybrid modeling. Quantum chemical description of the system – hydrogen and helium atoms. Many electron wave functions- second quantization. Reduced density matrices- Resolvents and Green's functions. Potential energy surfaces- geometry optimization- stationary points.

Electronic structure methods-independent particle models- SCF methods- energy of a Slater determinant- Koopman's theorem. The Basis set approximation- Restricted and unrestricted Hartree Fock- NDDO, INDO, CNDO methods. Parameterization- MINDO, AM1, PM3. Extended Huckel theory. Density Functional methods- orbital free DFT. Kohn – Sham theory (LCAO equations). Exchange- correlation functional. Linear scaling techniques. Pauli and Thomas – Fermi models. Hohenberg- Kohn theorems.

UNIT 3 Analytical Methods

Theory, Principles and general instrumentation of the following analytical techniques.
TG, DTA and DSC
AAS and ICP
Voltammetry- Cyclic voltammetry
XPS.

UNIT 4 Spectroscopy I

Ultraviolet-Visible Spectroscopy. Energy levels and selection rules, Influence of substituent, ring size and strain on spectral characteristics. Solvent effect; Stereochemical effect; Non-conjugated interactions. Spectral correlation with structure. Woodward-Fieser and Fieser-Kuhn rules. Introduction to Fluorescence spectroscopy

Infrared Spectroscopy. Fundamental vibrations, Characteristic regions of the spectrum. Structure-vibrational frequency correlations – effects of elctromeric and steric factors, IR spectroscopy as a method to identify functional groups present in a molecule.

Mass Spectrometry. Molecular ion, ion production methods (EI). Soft ionization methods: SIMS, CI, FAB, MALDI, PD, Field desorption, electrospray ionization, Fragmentation patterns, nitrogen and ring rules, rule of thirteen, McLafferty rearrangement, Applications. HRMS; formula mass and molecular formula, MS- MS, LC-MS, GC-MS.

UNIT 5 Spectroscopy 2

Magnetic Resonance Spectroscopy. Magnetic nuclei with special reference to 1H and 13C nuclei. Chemical shift and factors affecting chemical shift, chemical shift and magnetic equivalence, Spin-spin splitting, First order and higher order coupling, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, factors affecting geminal and vicinal coupling constants, long range coupling, coupling with other magnetic nuclei, Analysis of AX, AX2, AX3, A2X3, AB, ABC, AMX, ABX type of spin systems, Simplification non-first order spectra to first order spectra, shift reagents-mechanism of action, spin decoupling and double resonance, Introduction to 2D NMR techniques including COSY, HOMOCOSY and HETEROCOSY, HSQC, HMQC, HMBC, TOCSY (basics only, theory and detailed analysis not required), DEPT analysis and spectral editing. Electron spin resonance and its applications.

UNIT 6 Spectroscopy 2

Identification of structures of unknown organic compounds based on combined data from UV-Vis, IR, 1HNMR and 13CNMR spectroscopy (HRMS and Table of HRMS data may be provided).

References

1. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern, Singapore, 2nd ed., 1992.
2. V. Ramakrishnan, M. S. Gopinathan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996.
3. P. W. Atkins, Physical Chemistry 8th ed., W. H. Freeman, New York, 2006.
4. I. N. Levine, Quantum Chemistry, 6th ed., Pearson Education, London, 2008.
5. J. P. Lowe, Quantum Chemistry, 3rd ed., Academic Press, New York, 2008.

6. D. D. Fitts, Principles of Quantum Mechanics as Applied to Chemistry and Chemical Physics, CUP, Cambridge, New York, 2002.
7. M. Taketani, The Formation and Logic of Quantum Mechanics, Vol. I-III, World Scientific, New Jersey, 2001.
8. F. Jensen, Introduction to Computational Chemistry, 2nd ed., Wiley, New York, 2009.
9. R. Leach, Molecular Modeling, Principles and Applications, 2nd ed., Pearson Education, London, 2001.
10. A. Hinchliffe, Modeling Molecular Structures, 2nd ed., Wiley, New York, 2000.
11. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th ed., Saunders College Pub., 2007.
12. G. D Christian, Analytical Chemistry, 6th ed., John Wiley & Sons, 2007.
13. M. V. Cases, Principles of Analytical Chemistry, Springer, 2000.
14. D. L. Pavia, G. M. Lampman, G. S. Kriz, Thomson, Introduction to Spectroscopy: A Guide for Students of Organic Chemistry, 3rd ed., 2007.
15. Atta-Ur-Rahman, M. I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, New York, 1999.
16. L. D. Field, S.Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th ed., Wiley, 2008.
17. R. S. Drago, Physical Methods for Chemist, Saunders, 1992.
18. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed., McGraw- Hill, 1994.
19. F. Taber, Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, Oxford University Press, 2009.
20. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley and Sons, 1995.
21. R. M. Silverstein, G. C. Bassler, T. C. Morril, Spectroscopic Identification of Organic Compounds, John Wiley, 1991.
22. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill, 1988.
23. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.
24. Online spectral databases including RIO-DB.

ELECTIVE

CHE 4104 A – Chemical Instrumentation

(4 credit) 64 hours

UNIT 1- Analytical Methods

Classification of analytical methods – Types of Instrumental methods – Instruments for analysis – Data Domains – Non-electrical Domains – Electrical Domains – Analog Domains – Time Domains – Digital Domains – Detectors, Transducers and sensors. Sensitivity – Detection limit selectivity – Dynamic range.

UNIT 2 Atomic Spectroscopy

Sample atomization techniques – AAS – Theory and experimentation – Interference in AAS – Application. Inductively coupled plasma spectrometry – Theory and Instrumentation – Application

UNIT 3 Molecular Spectroscopy

UV – visible Absorption Spectroscopy – Beer's law Molar Absorptivities – Photometric Titration – Quantities Analysis – Instrumentation. Theory of IR spectrometry – IR sources and Transducers – Instrumentation.

UNIT 4 Potentiometry

REFERENCE Electrodes – Metallic indicator electrode – membrane electrodes – Potentiometric Sensors – ISFETS – Direct Potentiometry – Potentiometric Titrations – Instrumentation – Applications.

UNIT 5 Coulometry

Current – Voltage relationship during electrolysis . Coulumetry – Potentiostatic and Amperostatic – Theory and experimentation – Applications.

UNIT 6 Spectroscopy 2

DC Polarography - Supporting Electrolyte – Polorographic Maxima - half wave potential – Ilkovic equation – instrumentation and applications.

Cyclic Voltammetry – Theory and Experimentation – Applications – Voltammetric sensors.

UNIT 7 Separation Methods

GC – principles and instrumentation – application – HPLC – Principles & Instrumentation – Application

Ion exchange chromatography – Supercritical Fluid Chromatography.

UNIT 8 Thermal and Radiochemical Methods

Principles, experimentation and instrumentation of TG, DTA and DSC – Applications – Radiochemical Methods – Neutron activation analysis – Isotopic dilution – radiometric titration – Applications.

References

1. D.A. Skoog, F.J. Holler, T.A, Nieman Principles of Instrumental Analysis, Saunders College Pub., 1998.
2. H. H. Willard, L. L. Merritt, Jr., F. A. Settle, Jr., Instrumental Methods of analysis, 7th ed., CBS Publishers & Distributors, New Delhi,1998.
3. J. Mendham, R.C. Denney, J.D. Barner, M.J.K. Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6th ed., Pearson, 2008.
4. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th ed., Saunders College Pub., 2007.

ELECTIVE

CHE 4104 B – Inorganic Chemistry

(4 credit) **64 hours**

UNIT 1- Bonding in Metal Complexes

Crystal field theory-splitting of orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields-Ligand field stabilisation energy-John-Teller effect-Evidence for metal ligand overlap.

Molecular orbital theory of transition metal complexes-Molecular orbital energy level diagram for octahedral complexes with and without pi-bonding.

UNIT 2 Kinetics and Mechanism of Metal Complex Formation

Inert and labile complexes-crystal field activation energy-possible mechanisms for ligand replacement reactions Ligand exchange reactions in octahedral complexes of cobalt (III) and Square planar platinum (II), complexes – Trans effect-electron transfer processes.

UNIT 3 Catalysis by Transition Metal Complexes

Homogeneous catalysis involving organometallic compounds olefin hydrogenation, Wacker process, Ziegler-Natta process, Olefin metathesis-Monsanto process for the synthesis of acetic acid; heterogenization of homogeneous catalysis using insoluble and soluble polymeric supports.

UNIT 4 Electronic Spectra of Transition Metal Complexes

Charge transfer transition and d-d transition-selection rules and transition probabilities-effect of spin orbit coupling-Spectrochemical series of ligands-Term states for d ions-ergal diagrams-Tanable-Sugano diagrams-Calculation of Dq. Values with special reference to nickel complexes-Application of UV and visible spectroscopy in the study of metal complexes of first transition series.

UNIT 5 Magnetic Susceptibility of Transition Metal Complexes

Magnetic susceptibility measurements-Gouy Method-Magnetic moment-Orbital contributions to magnetic moment-spin orbit coupling-Temperature independent paramagnetism Application of magnetic moments to structure elucidation.

UNIT 6 Electron Spin Resonance

Instrumentation and sampling techniques-presentation of the spectrum-hyperfine splitting – Factors affecting the magnitude of g values-Zero field splitting and Kramers degeneracy-Nuclear quadrupole interaction-spin hamiltonian – Line widths in solid state EPR-Applications to metal complexes

UNIT 7 Solid State Chemistry

Point defects, line defects and plane defects-semiconductors-their use as Photoconductors, photovoltaic cells, rectifiers and transistors.

Super conductivity-occurrence of super conductivity BCS theory of super conductivity, (No Mathematical details needed) – magnetic properties of super conductors – High temperature superconductors.

UNIT 8 Bioinorganic Chemistry

Oxygen carriers and oxygen transport proteins-Haemoglobin, myoglobin and haemocyanin-co-operativity in haemoglobin-Iron storage and transport in biological systems-Ferritin and transforrin-Haeme proteins in redox reactions-Cyctochromes, peroxidases and catalyses-Vitamin B12. Nitrogenase-carboxy peptidase A.

References

1. J.E.Huheey, Inorganic Chemistry: Principles of Structure and reactivity, 4th ed., Harper Collin College Publishers, 1993. (For Unit-1)
2. F.A Cotton; Applications of Group Theory, Ind. ed, Wiley, New York, 1971. (for Unit 1)
3. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999. (for Units 1, 2, 6 & 7).
4. F.Basolo, R.G.Pearson, Mechanism of Inorganic reactions, Wiley, New York (for Unit-2).
5. K.F.Purcele, J.C.Kotz, Inorganic Chemistry, W.B. Sonders Company, Philadelphia. (for Unit 3).
6. R.S.Drago, Physical Methods in Chemistry, East West Edn. (Unit-4,5,6).
7. A.Earnshaw, Introduction to Magnetic Chemistry, Academic Press (Unit-5)
8. L.V.Azaroff, Introduction to Solids, Mc.Graw Hill, New York (Unit-7)
9. C.Kittel, Introduction to Solid State Physics, Wiley-Eastern, New Delhi (Unit-7)
10. R.W.Hay, Bio-inorganic Chemistry, Ellis Horwood Ltd., Chichester, 1984 (Unit-8)

CORE

CHE 4104 C – Quantum Chemistry

(4 credit)

UNIT 1- Postulates

64 hours

The postulates of Q.Mechanics Operators, eigenfunctions and eigenvalues Hermitian opoerators, orthonormal set, time dependent Schrodinger equation, stationary states, "Commutators and uncertainty principle DAM chapter 4.

UNIT 2 Exact Solutions I

The free particle in a box: wave functions, average momentum, illustration of the uncertainty principle. Harmonic Oscillator, eigenvalues and eigen functions, Normalisation of eigenfunctions and calculation of

<X>, <Px>, <X2> and <PX2 >

DAM Chapters 3 and 4

UNIT 3 Exact Solutions II

Particle in a three dimensional box, particle on a ring and on a sphere. The hydrogen atom (detailed solution is to be studied). DAM Chapter 5.

UNIT 4 Approximation Methods

Perturbation theory, first order correction to energy application to anharmonic oscillator, Variation theorem and its proof. Illustration by application to ground state of a harmonic oscillator linear variation method and the secular determinant.
DAM: Chapter 7

UNIT 5 Atoms

Atomic units, perturbation and variation methods for Helium atom, electron spin, Antisymmetry of wavefunctions. Slater determinants Hartree-forck equations, term symbols, hunds rules atomic spectra R-S coupling.

UNIT 6 Molecules I

Born-Oppenheimer appreoximation, VB for H_2 for H_2, the exchange integral single and triplet states of the Heitler London Theory. VB Theory and its relation to Lewis Formula, Hybridisation (sp. sp^2 and sp^3)

UNIT 7 Molecule II

MO theory for H^{2+} and H_2 ionic and covalent terms in the wavefunction, MOS for Homonuclei diatomic, electronic states of diatomic molecules.

UNIT 8 Molecular Spectroscopy

Wave functions for nuclear and electronic motion, separating out vibrational and rotational and translations parts, time dependent perturbation theory, selection rule for the rigid rotator and the harmonic oscillator, selection rule in electronic spectroscopy – Franck Condon Principle.
DAM : Chapter 10

References

The book referred to as DAM is: D.A.McQuarrie, Quantum Chemistry, Oxford University Press, 1983. The following books may be used as references:

1. P.W.Atkins, Molecular Quantum Mechanics, 2nd ed., Oxford University Press, 1983.
2. F.L.Pilar, Elementary Quantum Chemistry, McGraw Hill, 1980.

CHE 4104 D – Organic Chemistry - Terpenoids

(4 credit)

64 hours

UNIT 1

Introduction to terpene chemistry, classification of terpenoids, general biosyntheses of terpenoids, biosynthesis of mono, sesqui, di, ses, tri, tetre and poly terpenoids, Biosynthesis of Lanosterol, cholesterol and Vitamin A

UNIT 2

Monoterpenoids – Chemistry, including synthesis of industrially important monoterpenoide like pinene, menthol camphor, citral, geraniol, linalool, carenes, myrcine, citronellal etc.

UNIT 3

Sesqui terpenoids-Chemistry including synthesis of farnisol, santaloles, pachauli alcohol, cedrol longifolenes, caryophyllene alantalactone, Vetivones, Azulenes, dendrolasin, bisabolanes, eudesmol, cadinenes.

UNIT 4

Diterpenes-Chemistry including synthesis of Abietic acid, Gibberellins-with special emphasis to gibberllic acid, cembrene, Retenoids-with special emphasis on Vitamin A and related compounds.

UNIT 5

Sesterpenoids-general study of compounds-like Scalris ophiobolins and their synthesis. Triterpenoids – General Chemistry of Triterpenoids Chemistry including synthesis of alpha and beta – Amyrins, Lanosterol, Friedelin, Lupeol.

UNIT 6

Nortriterpenoids General study of the Chemistry abd synthesis of Limonoids with special reference to Limonin, Azadiractin, Nimbin, Malian triol and general study of triterpenoid antibiotics.

UNIT 7

Tetreterpenoids – General Chemistry and synthesis of cartenoids, Carotenes, lycopine and higher homolegues of cartenoids. Polyterpenoids – General study of polyoles Rubber and Gutta purcha etc.

UNIT 8

Metroterpenoids – Chemistry and synthesis of Vitamin K, Ubiquinones and related compounds, Vitamin E and related compounds. Alkaloids containing Isoprene units,l indole alkaloids, chemistry and biosyntheses of loganin and Secologanin and alkaloids derived from Secologanin lioke Ajmalicine, Emetine, Yohimbine, Reserpine and other alkaloids like Dendrobine, Garyfoline, Lycopodine, Solasodine and Tomatidine.

References

1. K.Nakanishi, Natural products Chemistry, Kodamniha Ltd. Vol. 1 and 3, Tokyo.
2. C.John Apsimon, The Total Synthesis of Natural Products, John Wiley & sone, Vol. 2, 4, 5, and 6.
3. L.Zecoeister, Progress in the Chemistry of Organic Naural Products, Springer – Verlag, Vol.48, NY (1985)
4. A, A. Newman, Chemistry of Terpenes and Terpenoids Ac. Press London (1972)
5. M.S.sporn, A.B. Roberts, The Retenoids, Academic Press Vol. 1 and 2, London (1972)
6. W.H.Sebrele and R.S.Harris, Vitamins, Academic Press Vol. 1 (1968) N.Y.
7. D.Barton and W.D.Ollis, Comprehensive Organic Chemistry, Pergamon Press, Vol. 5 (1979).
8. G.Ourisson etal, Teracyclic terpenes. Hermann Lparis (1964).

ELECTIVE

CHE 4104 E Organic Chemistry - Lipids

(4 credit)

UNIT 1

64 hours

Definition of lipids: Chemistry of fatty acids; their biosynthesis – Biosynthesis of triglycerids – Chemistry and biosynthesis of Phospholipids.

UNIT 2

General methods of synthesis of triglycerids and phospholipids-essential fatty acids their biosynthesis synthesis and biological activity.

UNIT 3

General Chemistry, biochemistry and pharmacology of prostaglandins – Derivatives of Arachidonic acids of biological importance; their biosynthesis and synthesis.

UNIT 4

Chemistry of sphingolipids and glycolipids – Chemistry of waxes

UNIT 5

Chemistry of steroids with special reference to chemistry and biosynthesis of cholestrol and lanosterol.

UNIT 6

Chemistry including synthesis and Biosynthesis of fat soluble vitamins.

UNIT 7

Chemistry of cell membrane the molecular component of cell membrane and its structure – Chemistry of lipoproteins a general study.

UNIT 8

Methods of analysis of lipids like fatty acids, triglycerides, phospholipids, oil soluble vitamins, essential fatty acids, prostaglandins and related compounds.

References

1. F.D. Gunstone, Topics in Lipid Chemistry, Vol 1, 2 & 3, Elek Sciences, London, 1972.
2. R. T. Holman, Profess in the Chemistry of fats and other lipids, Pergamon Press, Vol. 9, 1971.
3. Palee – Asciak, New Comprehensive Bio-Chemistry, Vol. 10, Glycolipids, Elseveir. Amsterda, 1982.
4. H.Weigandt, New Comprehensive Bio-chemistry, Vol. 10, Glycolipids, Elsevier, Amsterdam, 1985.
5. J.N.Hawthorne G.B. Ansell, Comprehensive Biochemistry, Vol.4, Elsevier, Amsterdam, 1982.
6. K.Nakanishi, Natural Products Chemistry, Kodanmsha Ltd., Vol, 2 and 3, Tokyo.

CHE 4104 F Organic Synthesis

(4 credit)

64 hours

UNIT 1

Reactive intermediates: carbocations, carbanions, carbenes, nitrenes, carbon radicals, radical ions and arynes. Nucleophilic- electrophilic- Radical substitution, addition and elimination reactions. Nucleophilic substitution at carbonyl carbon. Rearrangements to electron deficient carbon and nitrogen.

UNIT 2

Retrosynthetic analysis: The disconnection approach, designing a synthesis, FGI, Synthons, order of events, choosing a disconnection, synthesis of aromatic compounds, chemoselectivity in synthesis – one group C-X disconnections – alcohols, ethers, sulphides, alkyl halides, two group C-X disconnections – 1,1, 1,2 and 1,3-difunctionalozed compounds.

UNIT 3

C-C bond formations and disconnections

Reversal of polarity, protecting groups in synthesis, cyclisation and radical reactions, amine synthesis, 1,1 and 1,2-C-C disconnections, synthesis of alcohols, carbonyl compounds and carboxylic acids, synthesis of other compounds from alcohols, carbonyl compounds by one group C-C disconnections, enolate chemistry.

UNIT 4

Two group Disconnections

Diels-Alder reactions, 1,3-Difunctionalized and α,β-unsaturated carbonyl compounds, base catalysed reactions, 1,5-difunctionalized compounds, Michael addition and Robinson annulations, 1,2-Difunctionalized compounds, methods using acyl anion equivalents, 1,4- and 1,5-difunctionalized reactions.

UNIT 5

Retrosynthesis in action

Advanced strategies, retrosynthesis in industry, stereoselectivity and regioselectivity in synthesis, using alkenes, alkynes and nitro compounds in synthesis, reconnections, retrosynthetic analysis and synthesis – practice problems

References

1. J. March, Advanced Organic Chemistry-Reactions Mechanisms and Structure, 4th ed., John Wiley.
2. M. Smith, Organic Synthesis, McGraw-Hill, 2011.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry: Parts A and B: Reaction and Synthesis (Advanced Organic Chemistry / Part B: Reactions and Synthesis), Springer, 2007.
4. Online reference (www.organic-chemistry.org, for example)
5. S. Warren, Organic Synthesis – The Disconnection Approach, John Wiley and Sons 2004
6. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.
7. E. J. Corey, X.-M. Cheng, X, The Logic of Chemical Synthesis, Wiley, 1995.
8. K. C. Nicolaou, E. J. Sorenson, Classics in Total Synthesis: Targets, Starategies, Methods, Wiley 1996
9. J. H.Fuhrho, G. Li, Organic Synthesis- Concepts and Methods, Wiley-VCH 2003.

ELECTIVE

CHE 4104 G – Organic Chemistry *(Heterocyclic Compounds and Natural Products having Heterocyclic Systems)*

(4 credit)

UNIT 1 **64 hours**

Synthesis and reactions of condensed heterocyclic compounds with one N atom: indole, isoindole, quinoline and isoquinoline.

UNIT 2

Synthesis and reactions of six-membered heterocycles with more than one N atom: Pyrimidines, pyrazines, pyridazines, quinozolines, quinoxalines, purines and pteridines.

UNIT 3

Structure and synthesis of antibiotics containing heterocyclic systems: Penicillins, cephalosporins, cycloserine and mitomycin – C

UNIT 4

Structure, function and chemical synthesis of nucleosides nucleotides and nucleic acids.

UNIT 5

Alkaloids: General methods of isolation and structure determination, general reactions, biosynthetic route and biological activity of alkaloids.

Indole alkaloids: Structural determination and synthesis of reseroine, strychnine and heptaphylline.

UNIT 6

Quinoline and Pyrrolidine – Pyridine group alkaoids: synthesis and structural determination Cinchonine, quinine, nicotine, cocaine and atropine.

UNIT 7

Isoquinoline alkaloids: Structural determination and synthesis of papaverine, laudanosine, morphine, codeine and thebaine.

References

1. Barton, Ollis, Comprehensive Organic Chemistry, Vol. 4 & 5 Pergamon Press, Oxford 1979.
2. Katrikzy, Rees, Comprehensive Heterocyclic Chemistry, Vol. 2, 3, 4, 5, Pergamon Press, Oxford, 1984.
3. Manske and Holmes, The Alklaoids', Various Volumes, Academic Press, New York.
4. Pelletier, Alkaloids, Chemical and Biological Perspectives, John-Wiley and Sons, 1983.

CHE 4104 H Physical Chemistry *(Electrochemical Methods)*

(4 credit) **64 hours**

UNIT 1

The double layer: The Electrical Double layer, Gibbs absorption Isotherm, electrocapillary equation, experimental evaluation of surface excess. Models for double layer: Helmboltz, Gouy-Champman and Stern.

UNIT 2

Electrode potentials and Thermodynamics: Reversibility, Free Energy & Cell EMF. Physics of Phase potentials, Measurement of Potential differences. Electrochemical potentials. Liquid junction potentials (briefly) selective electrodes.

UNIT 3

Kinetics of Electrode reactions: The Tafel Equation, kinetic model based on electrochemical potentials, the exchange current, current-overpotential equation and its approximate forms, Microscopic theories of charge transfer kinetics (briefly).

UNIT 4

Mass Transfer: Derivation of general mass transfer equation, migration during electrolysis, effect of supporting electrolyte. Diffusion random walk model, Ficks laws, Boundary conditions in Electrochemical problems.

UNIT 5

Electroanalytical techniques I : Excitation signals used in electrochemical techniques – Voltammetry at a microelectrode – d.c. polarography, llkovic equation – pulse and differential pulse polarography.

UNIT 6

Electroanalytical techniques II : Chronopotentiometry, Chronoamperometry and chronocoulometry, coulostatic methods. Hydrodynamic methods, the convective diffusion equation, rotating disk electrode, current potential curves. Impedance techniques. Ac Voltammetry.

UNIT 7

Electrochemical Instrumentation – I : Circuit components-resistors, capacitors and inductors – their properties. Rate of current and potential changes in RC and RL circuits.

Response of RC and RL circuits to sinusoidal inputs-Voltage, current and phase relationship. High pass and low pass filters, resonant circuits.

Semiconductor diodes, diode characteristics, Biopolar transistors- electrical characteristics. Amplifiers employing transistors (simple circuit only) Emitter, follower amplifier differential amplifier and amplifiers with negative feed back.

UNIT 8

Electrochemical Instrumentation II : Rectifiers, filters and voltage regulators, operational amplifiers – general characteristics circuits employing – inverting circuit amplification and measurement of signals – Applications to mathematical operations.

Working principle of potentiostat and galvanostat.

References

For Unit I and IV – The syllabus is defined by the book by A.J. Bard and L.R. Faulkner, Electrochemical Methods, John Wiley. (1980).

For Units V to VIII : The same book but avoiding the mathematical details and chapter 3 of Skoog and West, Principles of Instrumental Analysis. 2nd edition, Saundern Collegbe, Philadelphia 1980.

The following books are also recommended.

1. Bockris and Reddy, Modern Electrochemistry, Vols. I & II Plenum Press.
2. I.H.Macbonald, Transient Technique in Electrochemistry, Plenum (1976).

ELECTIVE

CHE 4104 I – Adsorption and Catalysis

(4 credit)

UNIT 1 **64 hours**

Physisorption and chemisorption, Adsorption isotherms- Langmuir, Freundlich and BET, Thermodynamics of Adsorption, Variation of heat of adsorption with surface coverage, Activated and non activated adsorption, Kinetics of chemisorption- Langmuir Hinshelwood kinetics, Rideal Elay mechanism.

UNIT 2

Principles of green chemistry, Need for heterogeneous catalysis, Adsorption and catalysis, Activity and selectivity of catalysts, Factors influencing heterogeneous catalysis- particle size, diffusion limitations, electronic factors, catalyst poisoning, deactivation, regeneration.

UNIT 3

Fundamentals of photophysical and photochemical processes, Quantum yield, Quenching and sensitization, Stern Volmer plots, Photoinduced electron transfer reactions, Photovoltaics and Photoelectrochemical Properties, Semiconductor photocatalysis. Photocatalysis for environmental remediation/ energy applications- Water splitting and CO_2 reduction.

UNIT 4

Structural characterization: Spectroscopic Methods- General Principles and application of FTIR, Raman, Electronic and ESR spectroscopy- Identification of Catalytic sites.

UNIT 5

Surface Characterisation: Principle and application of XPS, XRD, SEM, TEM, AFM. Thermal Desorption techniques.

UNIT 6

Classification of materials based on pore size- micro, meso, nano. General properties of mesoporous materials, Synthetic routes- hydrothermal, solvothermal, sol-gel, micro emulsion, combustion. Nanomaterials- Quantum confinement, edge effect, top down and bottom up synthesis.

Synthesis, general properties and applications- Mesoporous carbon and silica, Carbon based nanomaterials- Graphene, Carbon nanotube, graphitic carbon nitride, Graphene quantum dots.

References

1. A. Clark, Theory of Adsorption and Catalysis, Academic Press, New York, 1970.
2. D.K. Chakraborthy, Adsorption and Catalysis by Solids, Wiley Eastern Ltd. 1990.
3. D.K. Chakraborthy, B. Viswanathan, Heterogenous Catalysis, Wiley Eastern Ltd. 2008.
4. J.M. Thomas, W.J. Thomas, Principles and Practice of Heterogeneous Catalysis, VCH Publishers Inc., New York, 1967.
5. J.R. Anderson and M. Boudart (Eds), Catalysis, Science and Technology, Vol 6, Springer- Verlag, Berlin Heildberg, 1984.
6. R.B. Anderson, Experimental Methods in Catalysis Research, Vol I, II, Academic press, New York, 1981.
7. G. Ertl, H. Knozinger and J. Weitkamp, Handbook of Heterogeneous Catalysis, Vol 2, Wiley-VCH, Weinheim, 1997.
8. W.N. Delgass, G.L. Haller, R. Kellerman and J.H. Lunsford, Spectroscopy in Heterogeneous Catalysis, Academic press, New York, 1979.
9. D.P. Woodruff and T.A. Delchar, Modern Techniques of Surface Science, Cambridge University Press, 1990.
10. J.W. Niemantsverdriet, Spectroscopy in Catalysis: an Introduction, VCH, NY, 1995.
11. N. J Turro, V. Ramamurthy, J. C Scaiano, Modern Molecular Photochemistry of Organic molecules, Viva Books, 2017.
12. M. Kaneko, I. Okura, Photocatalysis-Science and Technology, Springer 2002.
13. H. Kich, Semiconductor Photocatalysis- Principles and applications, Wiley VCH, 2015.
14. Francis. D'Souza, Karl. M. Kadish, Handbook of Carbon Nanomaterials Vol I, World Scientific Publishing Co. Pte. Ltd. 2011.

ELECTIVE

CHE 4104 J – Chemistry of Polymers

(4 credit)

UNIT 1 **64 hours**

Chemistry of polymers, concept of macromolecules. Historical development Classification and nomenclature. Structure – property – performance relationship. Synthesis of polymers. Different mechanisms of polymer synthesis. Step growth polymerization. Kinetics, mechanisms and molecular weight control. Linear vs nonlinear polymerization. Different techniques of polymerization.

UNIT 2

Free radical addition polymerization. Kinetics and mechanism. Chain transfer and molecular weight control. Thermal and photochemical radical generation. Steady state considerations. Ionic polymerization. Anionic and cationic mechanisms. Living polymers. Carbonyl polymerization. Copolymerization. Statistical approach to composition. Composition drift. Q-e scheme. Terminal copolymer model. Crosslinking. Gelation and gel point.

UNIT 3

Stereochemistry of polymers. Types of stereoisomers. Polymers with one and more asymmetric carbon atom. Architecture, orientation and conformation. Forces of steroregulation. Coordination polymerization. Zeigler – Natta and related catalyst systems. Polymerization of non polar alkene monomers. Olefin metathesis and ring opening. Optical activity in polymers. Three dimensional order and super structure.

UNIT 4

Characterization of polymers. Molar masses. Distribution and determination. Different methods of determination. Light scattering and gel permeation. Properties of polymer solutions. Thermodynamics. Average chain dimension. End-to-end distance. Freely jointed chain model. Flory – Huggins theory. Crystalline and amorphous state. Theories of polymer crystallinity – Thermal transitions of the crystalline and amorphous state. The elastomeric state. Rubber like elasticity. Network defects and resilience. Distribution function and statistical approach.

UNIT 5

Spectroscopy of polymers. Vibrational spectroscopy. Raman spectroscopy. Polarization effects. Raman and IR combination. High resolution NMR. Determination of

stereochemistry and copolymer composition. Two dimentional NMR. Determination of carbon connectivity. Solid state NMR. CP MAS technique. Pyrolisis mass spectrometry.

UNIT 6

Industrial polymers. Polyoletins. Polyethylene, polypropylene and related polymers. Polystyrene and styrene copolymers. PVC and related polymers. Manufacture and applications. Acrylic polymers. Poly (acrylic acid) and the acrylic ester polymers. Fluro polymers. Teflon and PVDF.

UNIT 7

Reaction polymers. polyamides and polyimides, Nylons. Aromatic polyamides. Polyesters. Unsaturated polyesters. Alkyd resins. PET and PBT. Polycarbonates. Phenolics and aminoplasts. Reactants and polymer types.

Polyurethanes. Reactants and additives. Chain extenders. Thermoplastic elastomers. Epoxies. Glycidyl ether of phenols and bisphenols. Epoxy diluents and curing agents.

UNIT 8

Speciality polymers. Liquid crystalline polymers. Main chain and side chain polymers. Chiral polymers. Photolabile and photosensitive polymers. Wave length dependent photorestructuring – application in photolithography and nonlinear optics. Functionalised polymers. Application in organic synthesis. Polymeric reagents and catalysts. Combinational synthesis.

References

1. F.W. Billmayer, A Text Book of Polymer Science, 3rd ed., John Wiley, New York, 1994.
2. R.J. Young, An Introduction to Polymer Science, 2nd ed., Chapman and Hall, New York, 1991.
3. J.M.J. Cowie, Polymers, Physics and Chemistry of Modern Materials, Blackie. Chichester, 1992.
4. H.J. Elias, Macromolecules Vol. I & II, 2nd ed., Academic Press, New York, 1991.
5. J.L. Koenig, Spectroscopy of polymers, ACS, Washington, 1992.
6. A Akelah and M. Moeit, Functionalised Polymers and their Applications, Chapman and Hall, New York, 1991.

ELECTIVE

CHE 4104 K – Pericyclic Reactions and Photochemistry

(4 credit)

UNIT 1 **64 hours**

Pericyclic reactions: Classification of Pericyclic reactions. Theory of Pericyclic reactions, Symmetry properties of Molecular orbitals, correlation diagrams, Woodward Hoffman rules.

UNIT 2

Analysis of pericyclic reactions using FMO method. Secondary orbital interactions, detailed study of intermolecular and Intramolecular Diels Alder reactions.

UNIT 3

Photochemistry: Electromagnetic spectrum, energy associated with UV-Vis region- laws of Photochemistry-interaction of light with matter, absorption and emission, Jablonski diagram, Frank-Condon principle, spin states and their interconversion, spin orbit coupling, energy transfer and electron transfer processes, excimers and exciplexs, Fluorescence and phosphorescence, Stern-Volmer analysis, introduction to photoinduced electron transfer reactions, generation of singlet oxygen, chemiluminescence.

UNIT 4

Photochemistry of organic molecules: cis-trans isomerizations, electrocyclic reactions and cycloadditions, reactions proceeding through bond dissociation – Norrish type 1 and type 2 reactions, photolabile protecting groups, photochemistry of aromatic compounds

UNIT 5

Rearrangements in the excited state: di-π-methane rearrangement, rearrangements involving enones, dienones, and cyclohexadienones, Barton's reaction.

References

1. Nicholas J. Turro, J. C. Scaiano, V. Ramamurthy, Modern Molecular Photochemistry of Organic Molecules, University Science Books; 1st ed., 2010.
2. T. H. Lowry, K. S. Richardson: Mechanism and Theory in Organic Chemistry, 3rd ed., Addison-Wesley.
3. F. A. Carey, R. J. Sundberg: Advanced Organic Chemistry, 3rd ed., Plenum Press.
4. N. S. Issacs: Physical Organic Chemistry, 2nd ed., John Wiley and Sons.
5. Woodward, Hoffmann: The Conservation of Orbital Symmetry, 5th ed., VCH Publishers.
6. I. Fleming, Molecular Orbitals and Organic Chemical Reactions, Wiley.

ELECTIVE

CHE 4104 L – Polymer Composites

(4 credit)

UNIT 1 **64 hours**

Manufacture, general properties and applications of butyl rubber, EPDM and EPM. Comparison of these rubbers with unsaturated elastomers with respect to chemical properties, vulcanization and uses. Study of other speciality elastomers like hypalon, silicones, polyurethanes, fluorocarbons, ethylene vinyl acetate copolymers etc. Manufacture, properties and applications of different thermoplastic elastomers.

UNIT 2

Additives used in rubber compounding: Curing systems, antidegradants, plasticizers, fillers, colourants, blowing agents etc.

UNIT 3

Machinery used for mixing, two roll mill, internal mixtures and continuous mixtures, extrusion technology, calendaring and different types of calendars.

UNIT 4

Moulding: Compression, transfer and injection moulding, different methods of vulcanization such as rotocure, autoclave open steam, high energy radiation etc.

UNIT 5

Introduction to composite materials- Classification, introduction to polymer composites- nano, micro and macro scales. Reinforcements-short fibre, long fibre and particulate fillers. Matrices-thermoplastics, thermosets and rubbers. Nano and microcomposites. Short and long fibre composites, treatment of reinforcements, polymer-filler interactions, use of coupling and bonding agents.

UNIT 6

Carbon nanotubes- single walled and multi walled - preparation, treatment and functionalisation. Salient features of polymer modification with carbon nanotubes, nanosilica and nanoclay. Organically modified layered clays. Various methods used for the incorporation of nanofillers in polymer matrix like solution mixing, latex stage mixing and melt mixing.

References

1. Rubber technology and manufacture – Blow C.M
2. High polymer lattices –D.C Blackley, Vols.111
3. Polymer processing – Mortin Jones
4. Rubber Technology Handbook – Hoffmann
5. Rubber processing – Freakly
6. G.Lubin-Handbook of composites-Van Nostrand(1982)
7. R.Krishnamoorti & R.A Vaia Polymer nano composites: Synthesis characterization and modeling , American Chemical Society (2002)

ELECTIVE

CHE 4104 M – Enzyme Technology

(4 credit)

UNIT 1

64 hours

Nomenclature and classification- structure of enzyme-primary, secondary, tertiary and quaternary, definition for cofactors, coenzymes, isoenzyme, apoenzymes, prosthetic group, turn over number- specificity of enzyme action- heat sensitivity - pH sensitivity.

Mechanism of enzyme action- models of enzyme-substrate reaction- enzyme kinetics- relationship between substrate concentration and reaction mechanism, Michael- Menton kinetics, Lineweaver -Burk equation

Enzyme Inhibition –Reversible – competitive, non –competitive, mixed- irreversible inhibition- mechanism and kinetics

UNIT 2

Principle of biocatalysts - reasons for immobilization

Methods of immobilization: adsorption, ionic bonding, covalent bonding - Inorganic carriers-Natural polymer as carriers-synthetic polymer as carrier- cross linking- matrix entrapment-membrane confinement- micro encapsulation- liposome techniques- enzymes in membrane reactors- various combined methods

UNIT 3

Activity as a function of temperature- determination of activation energies stability as a function of temperature- inactivation coefficient and half life- temperature optimum in long term process- influence of pH - influence of substrate concentration- influence of diffusion.

UNIT 4

Stirred reactor, loop reactors, bed reactors- packed bed, fluidized bed, membrane reactors, special form of reactors

UNIT 5

In analytical process: affinity chromatography, automatic analyzer, biochemical electrodes, enzyme thermistors, immuno methods- ELISA

In medicine: incorporeal enzyme therapy, extra corporeal enzyme therapy, artificial organs

In basic research: structural studies, properties of enzyme subunits, degeneration and regeneration, simulation of natural systems

Industrial application: waste water treatment, production of L-amino acids using L-aminoacylase, Lactose hydrolysis in milk, Fructose containing syrups.

References

1. Lehninger Principles of Biochemistry, David L. Nelson, Michael M. Cox, 5th ed., 2008.
2. W. Hartmeier, Immobilized Biocatalysts, An Introduction: Springer-Verlag, May 1988.
3. R. A Copeland Enzymes – A Practical Introduction to Structure, Mechanism and Data Analysis, Wiley-VCH, 3rd ed., 2002.
4. H. Bisswanger, Enzymes Kinetics – Principle and Methods, translated by Leonie Bubenheim, Wiley, 2002.
5. Illanes, Andres(Ed), Enzyme Biocatalysis-Principle and Applications, Springer-2008

ELECTIVE

CHE 4104 N Advanced Computational Chemistry

(4 credit)

UNIT 1

64 hours

Scope of computational chemistry, Introduction to molecular mechanics; comparison of popular force fields; performance of molecular mechanics, Molecular dynamics, the fundamental concepts of quantum mechanics - Schrödinger equation, Born-Oppenheimer approximation, potential energy surfaces, local and global minima, transition states, variational method, LCAO, Hartree-Fock theory, restricted HF calculations; open shell systems, ROHF and UHF calculations, Roothan–Hall equations, Koopmans theorem, HF limit and electron correlation,

UNIT 2

Basis sets, basis set approximation, Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, classification of basis sets – minimal, double zeta, triple zeta, correlation-consistent sets, core-valence sets, general contractions, EMSL basis set exchange, Semi empirical methods, post Hartree-Fock Method, Configuration interaction, Many-body perturbation theory, Coupled-cluster theory, Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF) theory, Density Functional Theory, Comparing the performance of electronic structure theories, Hybrid QM/MM

UNIT 3

Input of molecular structure, Z-matrix construction, single point energy calculations, geometry optimizations, Electronic Energy, Vibrational frequency analysis, symmetry analysis, zero-point vibrational energies (ZPVE's), distinguishing minima from transition states, Intrinsic reaction coordinate (IRC) analysis, transition barrier and activation energy, conformational energetics, reaction energetics, enthalpy of formation, bond dissociation energy, ionization energy, isomerization energy and barrier, potential energy surface, reaction mechanism, enthalpy, entropy and free energy changes for reactions, isodesmic reactions.

UNIT 4

Analysis of gaussian output files, dipole moment, multipole moments, polarizability, hyperpolarizability, and molecular electrostatic potential, partial atomic charges, thermodynamic properties, atomic spin, ionization potentials, electron affinities, infrared spectra and NMR spectra, use of graphics programs like Chemcraft, Molden in analyzing

Gaussian output data, identification and visualization of normal modes of vibration, calculation and interpretation molecular orbitals

UNIT 5

Determination of molecular properties using molecular mechanics, ab initio, semi empirical and DFT methods. Wave function analysis- population analysis. Geometry, Total energy, Dipole moment, vibrational frequency, Chemical Shifts. Determination of orbital energy gap – electronic spectral transitions. Application to materials- periodic boundary condition. Determination of polarizability and hyperpolarizability of organic molecules and polymers. Interaction with solvents and solvent effects- Onsager model. Solvatochromism.

References

1. C. J. Cramer, Essentials of computational Chemistry: Theories and Models, 2nd ed., John Wiley & Sons, 2004.
2. F. Jensen, Introduction to Computational Chemistry, 3rd ed., Wiley, New York, 2017.
3. A. R. Leach, Molecular Modelling Principles and Applications, 2nd ed., Pearson Education Limited, 2001.
4. A. Szabo, N. S. Ostlund, Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory, 2nd ed., Dover, 1996.
5. D. A. Mc Quarrie, Quantum Chemistry, 2nd ed., University Science Books, 2007.
6. I. N. Levine, Quantum Chemistry, 7th ed., Pearson, 2013.
7. F. A. Cotton, Chemical Applications of Group Theory, 3rd ed., Wiley, New York, 1990.
8. R.G. Parr, W. Yang, Density Functional Theory of Atoms and Molecules, Oxford University Press, Oxford, 1989.
9. D. Young, Computational Chemistry: A Practical Guide to Real World Problems, Wiley, New York, 2001.
10. A. Haaland, Molecules and Models: The Molecular Structures of Main Group Element Compounds, Oxford University Press, Oxford, New York, 2008.

ELECTIVE

CHE 4104 O – Chemistry of Nanomaterials

(4 credit)

UNIT 1 **64 hours**

Nanomaterials. Materials in the nanodomain. Zero, one and two dimensional materials. Particle size dependent change in properties of materials. Metals in the nanodomain - Gold and silver nanoparticles.

Properties and applications of nanomaterials. Core shell structures. Semiconductor nanoparticles. ZnO, ZnS, CdS and CdSe quantum dots - Electrical and optical properties.

UNIT 2

Synthesis of nanostructures – Chemical processes: Chemical precipitation and co-precipitation, polyol, and borohydrate reduction methods, Sol-Gel synthesis; Microemulsions synthesis, Hydrothermal, Solvothermal synthesis methods, Microwave assisted synthesis; Sonochemical assisted synthesis, Core-Shell nanostructure, Organic-Inorganic hybrid nanocomposites, Quantum dot (QDs) synthesis. Physical processes: Inert gas condensation, Arc discharge, RF- plasma, Plasma arc technique, Ion sputtering, Laser ablation, Laser pyrolysis, Ball Milling, Molecular beam epitaxy (MBE), Chemical vapour deposition (CVD) method. Template assisted synthesis, Catalyst assisted chemical vapour deposition (CCVD).

UNIT 3

Main group element Nanomaterials. Nano domains of Carbon. Fullerenes, carbon nanotubes, nanoribbons, nanorods, graphene, Graphene quantum dots. Synthesis, electrical and optical properties; Edge effect and Quantum confinement. Functionalization and its applications. Borophene, boron nanorods, boron nitride nanotubes - Properties and applications.

UNIT 4

Characterization of Materials. Microscopic techniques - TEM, SEM, FESEM, AFM - Principles, instrumentation and applications. Principles, instrumentation and application of Scanning probe microscopy (SPM/STM). Thermal methods - TG/DTG, DTA, DSC, X-Ray Diffraction.

UNIT 5

Optical spectroscopic methods. UV – visible Spectroscopy, Fluorescence Spectroscopy, XPS, Raman Spectroscopy - Principles, instrumentation and applications.

UNIT 6

Electroanalytical Techniques. Introduction - Current – Potential relationships, mass transfer by migration, convection and diffusion. Polarography – current – voltage curve. DME - components of polarographic current – diffusion current, supporting electrolyte, three electrode system, polarographic maxima. Half-wave potential – Instrumentation - Applications of Polarography. Pulse and differential pulse polarography. Ilkovic equation. Stripping analysis.

References

1. B. D. Fahlman, Materials Chemistry, Springer, Heidelberg, 2nd ed., 2011.
2. G. A. Ozin, A. C. Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials, RSC, UK, 2005.
3. C. Binns, Introduction to Nanoscience and Nanotechnology, John Wiley & Sons, 2010.
4. C. N. R. Rao, A. Müller, Anthony K. Cheetham, The Chemistry of Nanomaterials: Synthesis, Properties and Applications, Vol. 2, 2014.
5. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, Saunders College Pub., 8th ed., 2007.
6. J.R.Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd ed., 2006.
7. G. D Christian, Analytical Chemistry, John Wiley & Sons, 6th ed., 2007.
8. M. V. Cases, Principles of Analytical Chemistry, Springer, 2000.
9. H. H. Willard, L. L. Merritt, Jr., F. A. Settle, Jr., Instrumental Methods of Analysis, CBS Publishers & Distributors, New Delhi, 7th ed., 1998.
10. J. O'M. Bockris, A.K.N.Reddy, Modern Electrochemistry, Vols. I & II Plenum Publishers, London.