Syllabus of
Post Graduate Programs in
Applied Chemistry

(With effect from 2022-23 admitted batches)

Department of Chemistry

GIFT Autonomous, Bhubaneswar

An Autonomous Institution under UGC Act
Approved by AICTE, New Delhi
Affiliated to Biju Patnaik University of Technology, Odisha

Course Structure & Detailed Syllabus

M.Sc. in Applied Chemistry

(With effect from 2022-23 onwards)

Semester - I

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC101	Inorganic Chemistry	3-1-0	4
Theory	MCYC102	Organic Chemistry	3-1-0	4
Theory	MCYC103	Molecular Thermodynamics& Electrochemistry	3-0-0	3
Allied Elective	MCYE104	Introduction to Quantum Chemistry & Group Theory	3-1-0	4
Allied Elective	MCYE105	Molecular Spectroscopy	3-0-0	3
Practical	MCYC150	Inorganic Chemistry – I Laboratory	0-0-6	3
Practical	MCYC151	Physical Chemistry Laboratory	0-0-6	3
		Total	30	24

Semester - II

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC201	Spectroscopy and Magnetism in Inorganic Chemistry	3-1-0	4
Theory	MCYC202	Organic Syntheses	3-1-0	4
Theory	MCYC203	Physical Chemistry	3-1-0	4
Allied Elective	MCYE204	Analytical Techniques	3-0-0	3
Free Elective	MCYF205	Biochemistry	3-0-0	3
Practical	MCYC250	Organic Chemistry Laboratory	0-0-6	3
Practical	MCYC251	Inorganic Chemistry- II Lab.	0-0-6	3
Practical	MCYF252	Biochemistry lab.	0-0-3	2
			33	26

Subject Code – details

M – Master programme
CY- Chemistry
C – Core papers
E- Allied Elective
F- Free Elective
1st Digit – Semester number
2nd& 3rd digits – running number of the papers
(01 to 10 for theory papers. 50 and above for practicals)

Semester - III

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC301	Organometallic Chemistry	4-0-0	4
Theory	MCYC302	Chemistryof Drug Design	4-0-0	4
Free Elective	MCYF301	Environmental Chemistry	3-0-0	3
Free Elective	MCYF302	ChemicalSynthetic StrategyofAdvanced Materials&Nano materials	3-0-0	3
Free Elective	MCYF303	Computer programming for Chemistry	3-0-0	3
Practical	MCYC350	Advanced Physical chemistry lab.	0-0-6	3
Practical	MCYF351	Environmental Chemistry lab.	0-0-3	2
Practical	MCYF352	Computer programming lab.	0-0-3	2

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Semester - IV

Subject type	Subject code	Subject name	L-T-P	Credit
	MCYC401	Application of Advanced Instrumental Methods	3-1-0	3
	MCYC402	PolymerChemistry	3-1-0	3
	MCYC403	Solid State Chemistry	3-1-0	3
		Elective-I	3-0-0	3
		Elective-II	3-0-0	3
	MCYC-413	Project	0-0-12	8
	MCYC-414	Seminar		3

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Elective – I	**Elective - II**
MCYF 404- Nuclear Chemistry	MCYF 408- Frontiers in Organic Chemistry
MCYF 405- Organic Photochemistry &Synthesis of exotic molecules	MCYF 409- Frontiers in Inorganic Chemistry
MCYF 406- Supramolecular Chemistry	MCYF 410- Chemical Reaction Dynamics
MCYF 407- Chemistry of Natural Products	MCYF 411- Enzyme Reaction Mechanism and Kinetics
	MCYF 412- Single Electron Spectroscopy

1st Semester

MCYC101 INORGANIC CHEMISTRY

1. Structure and Chemical Bonding

VSEPR, Wash diagrams (tri atomic molecules), ds-ps bonds, Bent rule and energetics of hybidisation, some simple reactions of covalently bonded molecules.
OrganometallicChemistryof Lithium,Magnesium ,Si, Al, B: synthesis,structureandreactivity
Special emphasis on C_{60}andcarbonnanotubes:discovery,preparationandselectedreactions

2.TransitionMetalChemistry

Types ofligands, Structureandisomerismof transitionmetalcomplexes, Bondingin transitionmetal complexes–ValenceBond, CrystalField andMolecularOrbitaltheories, effectsof*d*-orbitalsplitting

3. Chemistry off-block elements

Position in the periodic table and applications, specialfeatures, lanthanidecontraction,coordinationnumber,structureandreactions

4. Metal-ligand Equilibria in Solution and inorganic reaction mechanism

Stability constants of metal complexes, Calculation of stability constants. and their applications
Stoichiometric and thermodynamic equilibrium constants, stepwise formation of complexes, formation functions. Mechanisms of substitution reactions of tetrahedral, square planar, trigonalbipyramidal, square pyramidal and octahedral complexes. Potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation , factors affecting the reactivity of complexes, Swain-Scott equation, Trans effect and its application to synthesis of complexes.
Molecular rearrangement processes: Electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reductant, chemical activation. Precursor complex formation and rearrangement, nature of bridging ligands, successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

SelectedTextBooks (Inorganic Chemistry):

1) Elschenbroich,C.;andSalzer,A.,Organometallics:A ConciseIntroduction,3rdEdn.1999.
2) Greenwood,N.N.;Earnshaw,A.,Chemistryof theElements,PergamonPress, 2ndEdn.,2002.
3) Douglas, B.;McDaniel, D.;andAlexander,J.,ConceptsandModels ofInorganic Chemsitry.3rdEdn., JohnWiley,NewYork.1993
4) Crabtree,R.H.The OrganometallicChemistry ofthe TransitionMetals,5thEdn.,John WileyandSons,2009
5) Shriver, D.F.;Atkins, P.W.andLangford,C. G. InorganicChemistry,3rdEdn.,OxfordUniversity,Oxford,1999.
6) Jolly,W.L.:ModernInorganicChemistry,2ndEdn., 1991.
7) Katakis, D. & Gordon, G. Mechanism of Inorganic Reactions John Wiley & Sons: N. Y (1987).
8) Langford, H. &.Gray, H. B. Ligand Substitution Processes W. A. Benjamin: N. Y. (1966).
9) Tobe, M. L. Inorganic Reaction Mechanisms F. C. Wadington, Ed., Thomas Nelson: London(1973).
10) J.E.Huheey,E.A.Keiter,R.L.Keiter&O.K.Medhi. *Principles ofStructureandReactivity* PearsonEducation(2006).
11) F. Basolo&R.G.Pearson,*Mechanismof InorganicReactions*, WileyEastern(1967).
12) F.A.Cotton,G.Wilkinson,C.A.Murillo&M.Bochmann.*AdvancedInorganicChemistry*(6th edition),JohnWiley(1999).
13) S.F.A.Kettle,*Physical InorganicChemistry*,Spectrum(1996).
14) R. G. Wilkins, The Study of Kinetics and Mechanism of Reactions of Transition Metal Complexes, Allyn & Bacon, Boston, 1974.
15) Robert B. Jordan, Reaction Mechansims of Inorganic and Organometallic Systems, Oxford University Press, 1998

MCYC 102 ORGANIC CHEMISTRY

UNIT –I

Nature of Bonding in Organic Molecules

Delocalised chemical bonding conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Armaticity in benzenoid and nonbenzenoid compounds, alternant and non-alternant hydrocarbons. Huckels rule,energy level of ⍰⍰molecular orbitals,annulenes,antiaromaticity,Ψ-aromaticity,homo-aromaticity,PMO approach.

Bonds weaker than covalent addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and Rotaxanes.

Stereochemistry

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution. Optical purity, enantiotropicand diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon(biphenyls, allenes and spiranes), chirality due to helical shape.

UNIT –II

Reaction Mechanism: Structure, Reactivity and Rearrengements

Types of mechanisms: SN2, SN1, mixed SN1 and SN2 and SET, SE1.

Kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates. Methods of determining reaction mechanisms, isotope effects, . Hard and soft acids and bases.

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

Effect of structure on reactivity- resonance and field effects, steric effect. Quantitative treatment. The Hammet equation and linear free energy relationships.substituent and reaction constants. Taft equation.

The NGP mechanism, NGP by π and σ bonds, anchimeric assistance.

Classical and nonclassicalcarbocations, phenonium ions, norbornyl systems. common carbocation rearrengements.

The SN1 mechanism. SN at an allylic, aliphatic trigonal and a vinyl carbon.

Reactivity effects of substrate structure, attacking nucleophile,leaving group and reaction medium. phase transfer catalysis and ultra sound. Ambient nucleophile, regioselectivit

Rearrengements

General mechanistic considerations- nature of migration. Migratory aptitude.memory effects. A detailed study of the following rearrengements

Pinacol-pinacolone, Wagner-Meerwein, Demjanov,Benzil-Benzilicacid,Favorskii,Arndt-Eistertsynthesis,Neber, Beckmann, Hofman, Curtius,Schmidt, Bayer-Villiger, Shapiro reaction.

UNIT-III

Aromatic Electrophilic Substitution Reactions

The Arenium ion mechanism, orientation and reactivity,energy profile diagrams.Theortho/para ratio,ipsoattack,orientation in other ring systems,quantitative treatment of reactivityin substrates and electrophiles.Diazoniumcoupling,Vilsmerreaction,Gattermann-Koch reaction

The SNAr, SN1, benzyne $S_{RN}1$ mechanisms.Reactivity effect of substrate structure,leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrengements.

Types of Free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate,neighbouring group assistance. Reactivity of aliphatic and aromatic substrates at bridgehead. Reactivity in the attacking radicals. The effects of solvents on reactivity.

Allylic halogenations (NBS), oxidation of aldehydes to carboxylic acids,auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free-radical rearrangement. Hunsdiecker reaction.

(NEW REACTION like Suzuki coupling,Bergmann synthesis,

Books Recommended (organic chemistry)

1.Advanced Organic Chemistry- Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J.Sundberg. Plenum
3. A guide book of mechanism in Organic Chemistry, Peter Sykes. Longman.
4. Structure and Mechanism in Organic Chemistry. C.K.Ingold. University Press
5. Organic Chemistry, R.T.MoririsonandR.N.Boyd. Prentice-Hall
6. Modern Organic Reactions, H.O.House. Benjamin
7. Principles of Organic Synthesis, R.O.C.Norman and J.M.Coxon. Blackie Academic and Professional
8. Pericyclic Reactions, S.M.Mukherji. Macmilan, India
9. Reaction Mechanism in Organic Chemistry, S.M.Mukherjii and S.P.Singh, Macmillan
10. Stereochemistry of Organic Compounds. D.Nasipuri. New Age International.
11. Stereochemistry of Organic Compounds. P.S.Kalsi. New Age International.
12. Organic Synthesis: Clayden, Greeves, Warren and Wouthers. Oxford University Press

MCYC103 MOLECULAR THERMODYNAMICS & ELECTROCHEMISTRY

Thermodynamics I: A brief survey of laws of thermodynamics
ThermodynamicsII: StandardStatesforGases,LiquidsandSolidsanditsApplications. Thermodynamics ofIonsinSolution,FreeEnergies,EnthalpiesandEntropiesofIonsin Solutions.ActivityandMeanActivityCoefficientsofElectrolytesandtheirDeterminations, Debye-HuckelLimitingLaw.Thermodynamics ofMixing–MixturesofVolatileLiquids–ideal and Real Solutions and Activities-Excess Functions. Thermodynamic Derivations of Phase Rule, ApplicationstoThreeComponentSystemsInvolvingSolidsandLiquids –Acetic Acid–Chloroform-Water, NaCl-Na_2SO_4-H_2O, NH_4NO_3-$(NH_4)_2SO_4$-H_2O.

Irreversible thermodynamics: Meaning and scope of irreversible thermodynamics, Thermodynamic criteria for non-equilibrium states, Phenomenological laws- Linear laws, Gibbs equation, Onsager's reciprocal relations, Entropy production- specific examples of entropy production, Non-equilibrium stationary states, Prigogine's principle of maximum entropy production, Coupled phenomena. Some important applications.
Transport phenomena: Diffusion coefficients, Fick's first and second laws, relation between flux and viscosity, relation between diffusion coefficient and mean free path, relation between thermal conductivity/viscosity and mean free path of a perfect gas, Einstein relation, Nernst-Einstein equation, Stokes-Einstein Debye equation (SED), Einstein-Smoluchowski-equation.

Electrochemistry-I: Debye Huckel-Onsager equation for the equivalent conductivity of electrolytes–experimentalverificationoftheequation–conductivityathighfieldandathigh frequency–conductivityofnonaqueoussolutions-effectofionassociationonconductivity. The electrode-electrolyte interface-electrical double layer-electro capillary phenomena- Lippmann equation–the Helmholz–Perrin–Guoy-Chapmann and Stern models, ElectrokineticphenomenaTiseliusmethodofseparationofprotonsofproteins-membrane potential.

Electrochemistry-II: Elecrodics- Mechanism of electrode reactions-polarization and overpotential–The Butler volmerequation for one step and multistep electron transfer reaction– significance of equilibrium exchange current density and symmetry factor- significance of transfer coefficient-mechanismof the hydrogen evolution reaction and oxygen evolutionreactions.Someelectrochemicalreactionsoftechnologicalinterest-corrosionand passivity of metals-construction and use of Pourbaixand Evans diagrams- methods of protection of metals from corrosion,Fuel cells - electro deposition.

TextBooks

1. S. Glasstone, Thermodynamics for chemists, Affiliated East WestPress,1965.
2. Atkins, P.W. 'Physical Chemistry', 6th Edn., Oxford University Press, 1998.

References

1. Electrochemistry by s.Glasstone
2. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, PlenumPress, 1970.
3.J.RajaramandJ.C.Kuriacose,ThermodynamicsforStudentsofChemistry,ShobanlalNaginChand Co, 1986.

MCYE104 INTRODUCTION TO QUANTUM CHEMISTRY AND GROUP THEORY

QuantumChemistry-I

Basic postulates of Quantum mechanics (a brief review). Operators in Quantum mechanics: Linear and Hermitian operators, Commutation of operators. Differential equations, partial differential equations, series solutions and special functions, linear vector spaces, transformation of coordinate matrix, representation of operators, eigenvalue problem, orthonormal sets, Fourier and Laplace transforms. Some exactly soluble problems. Simple harmonic oscillator problem. Calculation of various average values using ladder operators and recursion relations of Hermite polynomials. Angular momentum operators. Eigenvalues and eigenfunctions. First order time-independent perturbation theory for non-degenerate states. Variation theorem, variational methods and their applications. Ground and excited state of helium atom.

QuantumChemistry-II

Schrodingerequationforhydrogenatomanditssolution,theorigin of electronic quantum members and physical significance - radial probability density-significanceofmagnetic quantumnumberwithrespecttoangularmomentum.Hydrogen moleculeionandhydrogenmolecule-Paulisexclusionprinciple.Termsymbolsforelectronic stateinatoms–LSandJJcoupling.BornOppenheimerapproximation,Variational treatment of hydrogen molecule ion. Mullikendesignation ofmolecularorbitals, wavefunctionsformanyelectronatoms–Hartres–Fock SCF method, Slater Orbitals.

Group Theory-I

Symmetry Elements and Symmetry Operations, Point Groups, Representation of Groups, Reducible and Irreducible Representation; Character Tables, OrthogonalityTheorem– Its Consequences.

TextBooks (Quantum Chemistry and Group Theory)

1. I. N. Levine, 'QuantumChemistry', 4th Edn., Prentice Hall India, 2001.
2. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill 1994.
3. M.S.GopinathanandV.Ramakrishnan,GroupTheoryinChemistry,VishalPublishers,1988.
4. MethodsofMolecular Quantum Mechanics byP.W. Atkins.
5. Cotton,F.A.ChemicalApplicationsofGroupTheory,3rdEdn., JohnWileyandSons, 2003.
6. Physical Chemistry: A Molecular Approach byD.A.McQuarrieandJ.D.Simon
7. D.A.McQuarrie. *QuantumChemistry*,Viva BooksPvtLtd(2003)
8. Jack Simons, Introduction to Theoretical Chemistry, Cambridge University Press, 2003.
9. P.W.Atkins.*MolecularQuantumMechanics*,Oxford UniversityPress (1986)

MCYE105 MOLECULAR SPECTROSCOPY

Basic elements of spectroscopy, Interaction of Radiation with matter,Time dependent perturbation. Einstein coefficients. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Atomic spectra: Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legandre polynomials). Spectra of complex atoms. Zeeman and Stark effects.

Introduction to molecular spectroscopy: Rotational spectroscopy of diatomic molecules. Rigid rotor approximation. Determination of bond lengths and/ or atomic masses from microwave spectral data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First order Stark effect.

Vibrational spectroscopy:homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones and combination bands. Introduction to normal coordinate analysis.

Dissociation energies from vibrational spectral data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect.

Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules.

Raman spectroscopy: Stokes and anti-Stokes lines. Polarizability of molecules. Rotational and Vibrational Raman spectroscopy. Selection rules. Polarization of Raman lines.

Electronic spectroscopy: Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N_2) and simple polyatomic molecules (H_2O, formaldehyde). Adiabatic and vertical ionization energies. Koopmans' theorem. Qualitative ideas of solvent effects- viscosity, polarity, hydrogen bonding.

NMR: Generalintroductionanddefinition;chemicalshift;spin–spininteraction;shielding mechanismof measurement;chemicalshiftvaluesandcorrelation forprotonsbondedto carbons[aliphatic;olefinic;aldehydicandaromatic]andothernuclei[alcohols;phenols; enols;acids;amines;amidesandmercaptans];chemicalexchange;effectofdeuteration; complex spin-spin interaction between two; three; four; and five nuclei [first order spectra];virtualcoupling.Stereochemistry;hinderedrotation;Karpluscurvevariationofc ouplingconstantwithdihedral angle.

Electron Spin Resonance: Electron spin and Magnetic moment , Resonance condition in ESR and significanceof'g'value.ESRspectraoforganicfreeradicals,McConnelrelation ,ElectronExchangereactions, applicationsofESR.

Principles of Mossbauer spectroscopy: basic principles, achirality of nucleus, Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination.

Books (Molecular Spectroscopy)

1. PhysicalMethodsin Chemistry,RS Drago,2ndedn., Saunders,1992.
2. BasicOne-andTwo-DimensionalNMRSpectroscopy,H.Friebolin,VCH,1991.
3. SpectroscopicMethodsin OrganicChemistry,D.H.Williams andI.Fleming,4thed., 1988.
4. SpectrometricIdentificationofOrganicCompounds,R.M.Silverstein,G.C.BasslerandT .C. Morrill,JohnWiley& Sons,NewYork,5th Ed.1991.
5. *ElectronParamagneticResonance,ElementaryTheoryandPracticalApplications,*Weil,J ohn A,J.R.Bolton, andWertz,J.E,Wiley-Interscience,New York,(1994).
6. StructuralMethodsinInorganicChemistry,E.A.V.Ebsworth,D.W.H.Rankin,&S.Cradock , 2nd Ed.1991,CRC Press,Boca Raton, Florida,
7. Principles of Fluorescence Spectroscopy, Lackowicz,Plenum Press,(New York,1983)
8. Bernath, SpectraofAtomsandMolecules, 1995.
9. Bunker& Jensen,MolecularSymmetry &Spectroscopy,1998.
10. D.W.WilliamsandFlemming,Spectroscopicmethodsoforganiccompound.
11. J.R.Dyer.Applicationofabsorptionspectroscopyoforganic compounds.
12. Jackman andSterneil, ApplicationofNMR spectroscopy
13. J.D.Roberts,Nuclearmagneticresonance(J. Wiley)
14. JafeeandOrchin,Theoryand applicationof U.V,
15. BeynonJHet.al , Themassspectraoforganicmolecules.
16. WillardMerritt andDean.Instrumentalmethodsofanalysis

MCYC150 INORGANIC CHEMISTRY LABORATORY

I.Semi-microAnalysisoftransitionmetalandrareearthmetalionsina mixture byusing Spot technique.
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II.Preparation of the following (any two)
l.Chrome alum2. Copper (I) chloride 3. Tris(thiourea) copper (I) complex 4. Potassium tris(oxalato) aluminate (III) 5. Hexaaminecobalt (III) chloride 6. Tetraaminecopper (II) sulphate.

Estimationofiron/ copper/ nickelinminutequantitiesbyUV-Visspectrophotometry
Principlesofcolorimetricanalysis:determinationof ironcontent of anunknownsample.

Preparationofhexamminenickel(II)chloride:estimationofammoniaandnickelby titrimetricandgravimetricmethodsDeterminationofcomposition of a complex usingsimple techniques

Potassium*tris*-oxalatoferrate(III):synthesis,analysisandphotochemistrySynthesisofthe complexandits utilizationinblue-printingexperiment

SelectedTextBooks:

1. Elias,A.J.,ACollectionofInterestingGeneralChemistryExperiments,UniversitiesPress, (India)Pvt.Ltd.,2002.
2. Roesky, H. W.; Möckel, K., Chemical Curiosities: spectacular experiments and inspired quotes,VCH,1996.

Hand-outspreparedfor thelaboratoryexperiments:collectionsfrom variousliteraturesources

3. l.G.,Svehla,'Vogel'sQualitativeInorganicAnalysis',6thEdn.,OrientLongmanNew Delhi,l987.
4. V.V., Ramanujam , 'Inorganic Semi-micro Qualitative Analysis', 3rd Edn., National PublishingCompany,Madras,l990.

1st semester

MCYC151 PHYSICAL CHEMISTRY LABORATORY

1. pH metry / conductometry / potentiometry and precipitation titrations
2. Spectrophotometricdeterminationof theacid dissociationconstant .
3. Inversion of sucroseusing polarimeter.
4. Determinationofcriticalmicellerconcentration of surfactants..
5. Polarizabilityfromrefractiveindexmeasurements.
6. Composition of acomplexby Job's method.

TextBooks

1. D.P.Shoemaker,C.W.Garland&J.W.Nibber,,'ExperimentsinPhysicalChemistry', McGraw Hill 5th Edn., 1989.
2. A. I. Vogel, 'Text book of Practical Organic Chemistry',5thEdn. ELBS, London , l989.

References

1. B.B.Dey,andM.V.Sitharaman,'LaboratoryManualofOrganicChemistry'Revisedby T.R.Govindachari, Allied PublishersLtd., New Delhi. 4th Revised Edn. l992.

2nd semester

MCYC201 SPECTROSCOPY AND MAGNETISM IN INORGANIC CHEMISTRY

Raman spectra and selection rules, polarized and depolarized Raman lines, resonance Raman spectroscopy, use of symmetry to determine the number of active infrared and Raman lines, rotational fine structure in gas phase IR. Nonresonance overtones and difference bands. Application of Raman and Infrared selection rules to the determination of inorganic structures, bond strength frequency shift relations, changes in spectra of donor molecules on coordination, change in symmetry on coordination.

Magnetism: Types of magnetic behaviour, magnetic susceptibilities, Pascal's constants, paramagnetism in experimental simple systems .van Vleck's equation, its derivation and its applications. Spin-orbit coupling and susceptibility of transition metal ions and rare earths; magnetic moments of metal complexes with crystal field terms, antiferromagnetism and ferromagnetism of metal complexes, Curie-Weiss law, superparamagnetism. High and low spin equilibria.

Mass spectroscopy: Experimental arrangements and presentation of spectra, molecular ions, appearance and ionization potential, fragmentation, ion reactions and their interpretation, effect of isotopes on the appearance of a mass spectrum, molecular weight determination, thermodynamic data. Application of mass spectroscopy to inorganic compounds.

Electronic spectroscopy: Vibrational and electronic energy levels in a diatomic molecule, potential energy level diagram, Morse function, selection rules, spin orbit and vibronic coupling contributions, mixing of d and p orbitals in certain symmetries.

Nuclear magnetic resonance spectroscopy: Application of chemical shifts, signal intensities and spin-spin coupling to structure determination of inorganic compounds carrying NMR active nuclei. Effect of fast chemical reactions, coupling to quadrupolar nuclei, NMR of paramagnetic substances in solution, nuclear and electron relaxation time, contact shift, pseudo contact shift.

Electronic paramagnetic resonance spectroscopy: Hyperfine splitting in EPR spectroscopy.

Recommended Texts:

1. Ebsworth, E. A. O. Structural Methods in Inorganic Chemistry Blackwell Scientific Publications (1991).
2. Drago, R. S. Physical Methods in Chemistry W. B. Saunders Co.: U.K. (1977).
3. Carrington, A. & McLachlan, A. D. Introduction to Magnetic Resonance Chapman & Hall: N.Y. (1983).
4. Mabbs, F. E. &Machin, D. J. Magnetism and Transition Metal Complexes Chapman and Hall: U.K. (1973).

MCYC202 ORGANIC SYNTHESES

UNIT I

Disconnection Approach

An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, umplong approach, cyclisation reactions, amine synthesis.

Oxidation

Introduction. Different oxidative processes.

Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated andunactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulfides. Oxidations with ruthenium tetraoxide, iodobenzenediacetate and thallium (III) nitrate.

Reduction

Introduction. Different reductive processes.

Hydrocarbons- alkenes, alkynes and aromatic rings.

Carbonyl compounds- aldehydes, ketones, acids and their derivatives. Epoxides, Nitro,nitroso, azo and oxime groups. Hydrogenolysis.

UNIT II

Protecting Groups

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

One Group C-C Disconnection

Alcohols and carbonyl compounds, regioselectivity, Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Two Group C-C Disconnections

Diels-Alder reaction, 1, 3–difunctionalised compounds, α, β- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Micheal addition and Robinson annelation.

UNIT III

Ring Synthesis

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis.

Synthesis of some Complex Molecules

Application of the above in the synthesis of following compounds. Camphor, Vitamin D and Cortisone.

UNIT-IV

Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motion,4n,4n+2 and allylsystems.Cycloadditons-antarafacial and suprafcial additions, 4n and 4n+2 systems,2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropicrearrengements- suprafacial and antarafacial shifts of H, sigmatroic shifts involving carbon carbon moieties,3,3- and 5,5- sigmatropicrearrengements. Claisen, Cope and aza-Cope rearrengements. Fluxonaltautomerism.Ene reaction

Books Recommended

1. Designing Organic Synthesis, A programmed introduction to synthon approach, S. Warren, Wiley.
2. Organic Synthesis-concept, Methods and Starting Materials, J. Fuhrhop and G. Penzllin, VCH, Weinheim, Germany.
3. Some Modern Methods of Organic synthesis, W. Carruthers, Cambridge Univ. Press.
4. Modern Synthetic Reactions, H. O. House, W. A. Benjamin
5. Advanced Organic Chemistry: Reactions, Mechanisms and Structure, J. March, Wiley.
6. Principles of Organic synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
7. Advanced Organic Chemistry Part B, F. A. Carey and R. J.Sundberg, Plenum Press.
8. Organic Chemistry: The disconnection approach , S. Warren, John Wiley and Sons.

MCYC 203 PHYSICAL CHEMISTRY

Kinetics: Complexreactions–opposing,parallelandconsecutivereactions.Theories of reaction rates: Collision theory. Potential energy surfaces (basic idea). Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment). Solution kinetics: Factors affecting reaction rates in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant. Secondary salt effects, isotope effect,Kramerstheory. Molecularbeamexperiments.Diffusionlimitedreactions. Chain reactions–linearreactions, branching chains– explosion limits; Rice Herzfeld scheme.
Enzymecatalysis–ratesofenzymecatalysedreactions–effectof substrate concentration, pH and temperature–determination of Michaelis-Menten parameters.

Surface phenomena: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature, Factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization, solubilization, microemulsions, reverse micelles, surface films (electrokinetic phenomena), catalytic activity at surfaces. Electrode/ electrolyte interface; electrical double layer, electrode kinetics, Nernst equation.

Photochemistry: Absorption of light and nature of electronic spectra, electronic transition, Frank-Condon principle, selection rules, laws of photochemical equivalence, photodissociation, predissociation, photochemical reactions: photoreduction, photooxidation, photodimerization, photochemical substitution, photoisomerization. Photochemistry of environment: Greenhouse effect.

Photo physicalphenomena: Electronicstructureof molecules, molecularorbital,electronicallyexcited singletstates,designationbasedonmultiplicityrule,life timeofelectronicallyexcitedstate,constructionofJablonskidiagram,electronic transitionsandintensityofabsorptionbands,photphysicalpathwaysofexcited molecular system(radiativeandnon-radiative),promptfluorescence,delayedfluorescence, and phosphorescence, fluorescence quenching: concentrationquenching,quenchingbyexcimerandexciplexemission,fluorescenceresonanceenergytransferbetweenphotoexciteddonorandacceptorsystems.

Recommended Books (**Physical Chemistry**)

1. P.W.AtkinsandJulio dePaula:PhysicalChemistryI.N.Levine:PhysicalChemistry
3. D.A.McQuarrieandJ.D.Simon:PhysicalChemistry- AMolecularApproach
4. D.A.McQuarrie,StatisticalMechanics
5. H.B.Callen:ThermodynamicsandanintroductiontoThermostatistics
6. DavidChandler:IntroductiontoModernStatisticalMechanics
7. R.S.Berry,S.A.RiceandJohnRoss :PhysicalChemistry
8. R.J.Silbey,R.A.Alberty,andM.G.Bawendi,PhysicalChemistry
9. Photochemistry–J.G.CalvertsandJ.N.Pitts,John-Wiley&Sons
10. FundamentalsofPhotochemistry-K.K.Rohatgi-Mukharjii, WileyEastern
11. Introductionto Photochemistry-Wells
12. Photochemistryof solutions-C.A.Parker, Elsevier
13. ChemicalKinetics-K.J.Laidler,pearsonEducation,2004
14. NicholasJ.Turro,ModernMolecularPhotochemistry
15. J.R.Lakowicz, PrinciplesofFluorescenceSpectroscopy

MCYE204 ANALYTICAL TECHNIQUES

Ultraviolet Spectroscopy: Fundamental of electronic transitions, selection rules for allowed and forbidden transitions. Studiesofconjugated andextended conjugated systemsetc.Woodward rules.Electronicspectraoftransitionmetalcomplexes.

InfraredSpectroscopy: identification of the criteria for IR active character of molecules, Identificationof functionalgroups,hydrogenbonding etc.,metalligandvibrations.Characterization of metal –oxygen bonding in metal oxide nanoparticles.

NuclearMagneticResonanceSpectroscopy: Applicationof^{1}Hand^{13}CNMR spectroscopy includingCOSY,NOESY,NOEtechniquesinthestructuraldeterminationof complexorganic systems. Applicationinconformationalanalysis.MultinuclearNMRof variousinorganicand organometalliccompounds.

Mass Spectrometry: Fragmentationand rearrangements (includingMcLaffertyrearrangement)of differentclassesoforganicmolecules.Isotopeeffectsetc. and basics of HRMS, and its necessity in organic synthetic chemistry field.

ElectronSpinResonanceSpectroscopy: AnalysisofESRspectra ofsystemsinliquidphase, radicalscontainingsingleset,multiplesetsofprotons,triplet groundstates.Transition metalions. Doubleresonance techniques: ENDOR inliquid solution, ENDOR in powers and non-oriented solids. EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Application of Photo Electron Spectroscopy (PES), ESCA and Auger spectroscopy to the study of surfaces.

CDspectroscopy:CDofpolypeptidesandnucleicacids,InducedCD,magneticcircular dichroism.

Electro-analytical techniques: Heterogeneous electrontransfer and concept of capacitive and faradiccurrent.Cyclicvoltammogram.Instrumentation:three-electrodepotentiometerand electrodes.

Measurements andanalyses of the voltammograms. Differential pulsevoltammetryand coulometry.Applicationofcyclic voltammetryininorganicandorganic chemistry.

Fluorescence spectroscopy: Fluorescence energy transfer and its applications to measurementof distancesin molecules.

Thermal Analysis: Thermogravimetric analysis (TGA) and its applications to inorganic and polymer material characterization. Differential scanning colourimetry (DSC) and its application to inorganic materials.

Chromatography: Fundamental of chromatographic separations, retention time, distribution ratio, K factor.

High Performance Liquid Chromatography (HPLC) its application to organic compounds. Gas Chromatography (GC) and its applications to synthesis and environmental fields (with one example each).

Books (ANALYTICAL TECHNIQUES)

1. PhysicalMethodsin Chemistry,RS Drago,2ndedn., Saunders,1992.
2. Carbon-13NuclearMagneticResonanceSpectroscopy,G.C.Levy,R.L.LichterandG.L.Nelson,Wiley,1980.
3. NMRSpectroscopy- AnIntroduction,H. Gunther,JohnWiley,1980.
4. BasicOne-andTwo-DimensionalNMRSpectroscopy,H.Friebolin,VCH,1991.
   SpectroscopicMethodsin OrganicChemistry,D.H.Williams andI.Fleming,4thed., 1988.
   SpectrometricIdentificationofOrganicCompounds,R.M.Silverstein,G.C.Basslerand T.C. Morrill,JohnWiley& Sons,NewYork,5th Ed.1991.
5. *ElectronParamagneticResonance,ElementaryTheoryandPracticalApplications,*Weil ,John A,J.R.Bolton, andWertz,J.E,Wiley-Interscience,New York,(1994).
6. StructuralMethodsinInorganicChemistry,E.A.V.Ebsworth,D.W.H.Rankin,&S.Cradock, 2nd Ed.1991,CRC Press,Boca Raton, Florida,
7. CircularDichroism: PrinciplesandApplications,Nakanishi,K.,Berova,N.,Woody,R.W., Eds.;VCHPublishers,Inc.:NewYork,1994.
8. Principles ofFluorescence Spectroscopy, J. Lackowicz,Plenum Press, (NewYork1983)ElectrochemicalMethods-FundamentalsandApplications,A.J.BairdandL.R.Faulkner, Wiley,1980.

MCYF205 BIOCHEMISTRY

Module-I **(20Hr.)**

Introduction to Biomolecules:
Structure and Function of Carbohydrates: Monosaccharide, Oligosaccharides, Polysaccharides (Starch, Glycogen, Cellulose), Optical Isomerism;
Structure and Function of Lipids: Saturated and Unsaturated Fatty Acids, Triacylglycerols, Phosphoglycerides, Sphingolipids, Waxes and Sterol;
Structure and Function of Proteins: 20 Amino acids, Peptide bond, Hierarchy of protein architecture, Ramachandran Plot, 3-D structure;
Structure and Function of Nucleic Acids: DNA, RNA, Double Helix Model of DNA, Denaturation and Renaturation DNA;
Structure and function of Hormones, Minerals and Vitamins; Bio-complexes: Nucleoproteins, Glyco-proteins, Lipoproteins and Vitamin complexes.

Module-II **(10Hr)**

Principle of Bioenergetics: Bioenergetics and Thermodynamics; Phosphoryl group transfer and energy currency-ATP; Biological Oxidation and reduction reactions
Metabolism-I: Introduction to metabolic processes;
Metabolism of Carbohydrates: Glycolysis, TCA Cycle, ETS and Oxidative Phosphorylation, HMP pathway, Gluconeogenesis , Glycogen metabolism;
Metabolism of Lipids: Anabolism (Saturated and Unsaturated), Catabolism (α- Oxidation, β-Oxidation) and Energetics of lipid metabolism;
Metabolism Of Nucleic Acids: Catabolism and anabolism of purine and pyrimidine nucleotides.

Module-III **(10Hr)**

Metabolism-II: Metabolism of proteins: Properties of Amino acids, Biosynthesis of amino acids (Valine, Serine, Histidine and Glutamic Acid); Protein Catabolism (Genetic code and Protein synthesis); Protein Turnover, Protein Targetting.
Enzymes: Properties of Enzyme, Classification of Enzymes, Mechanism of enzyme action, Kinetics of of enzyme action, Activation energy, Enzyme Inhibition, Coenzyme, Apozyme and Holozyme

Text Book

1. Principle of Bio-Chemistry – Lehinger, Nelson and Cox
2. Biochemistry of Biochemistry by L. Stryer
3. Fundamentals of Biochemistry – Voet&Voet
4. Biochemistry by Zubay.
5. Biochemistry, C.B.Powar&G.R.Chatwal, Himalaya Publishing House.
6. Biochemistry, Rastogi, Tata McGraw Hill.

MCYC250 ORGANIC CHEMISTRY PRACTICAL

Qualitative Analysis

Identification of organic compounds, separation, purification and identification of compounds of binary mixture using TLC and column chromatography. Chemical tests: IR spectra to be used for functional group identification.

Isolation of active natural products (caffeine, clobe oil etc.)from natural sources.

Preparation of paracetamol.

Application of steam distillation.

Preparationofo-iodobenzoicacidfromanthranilicacid;furoicacidfromfurfural;thiamine catalysedbenzoincondensation;preparationof benzilfrom benzoin;

Estimation of Phenol, Aniline, Ascorbic Acid.
Estimation of glucose by Fehling's method & Bertrand's method.
Isolation of natural products (carcumene/caffeine/clove oil) from natural occurring substances
Application of steam distillation
Prepartion of paracetamol.

Text Book

1. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson & M. Miller, Printice Hall.

2. Systematic Qualitative Organic Analysis, H. Middleton, E. Arnold (publisher)

3. Hand Book of Organic Analysis, Qualitative & Quantitative, M. T. Clarke, E. Arnold (publisher)

4. A. I. Vogel, 'Text book of Practical Organic Chemistry',5thEdn. ELBS, London, l989.
5. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.

MCYC251 INORGANIC CHEMISTRY - II PRACTICAL

I.Semi-microanalysis:Analysisofmixturecontainingtwocommoncationsandanytwoof the following less familiar cations.Ti, W, Mo, V and U .

Preparation of Inorganic complexes & their charaterisation by different classical and spectroscopic techniques.

Preparation of diamagnetic and paramagnetic main-group and transition-metal acetylacetonates
Synthesis,isolationandspectroscopiccharacterizationof thecomplexes

Spectrophotometric determinationof phosphate: estimation of phosphate in cola drinks
Determinationofconcentrationof phosphatesapplyingBeer-Lambertlaw

TextBooks

1. l.G.,Svehla,'Vogel'sQualitativeInorganicAnalysis',6thEdn.,OrientLongmanNew Delhi,l987.
2. V.V., Ramanujam , 'Inorganic Semi-micro Qualitative Analysis', 3rd Edn., National PublishingCompany,Madras,l990.
3. Elias,A.J.,ACollectionofInterestingGeneralChemistryExperiments,UniversitiesPress (India)Pvt.Ltd.,2002.
4. Roesky, H. W.; Möckel, K., Chemical Curiosities: spectacular experiments and inspired quotes,VCH,1996.

2nd semester/ MCYF 252 BIOCHEMISTRY LAB

1. Spectroscopic/Colorimetric estimation of protein using Lowry's method
2. Spectroscopic estimation of DNA using DPA method
3. Spectroscopic estimation of RNA using Orcinol method
4. Estimation of Iodine number and saponification value of fatty acids
5. Separation of amino acids by paper chromatography
6. Separation of sugars by thin layer chromatography
7. Separation of proteins by SDS-PAGE.
8. Assay of Enzyme acivity: Protease from bacteria.
9. Assay of enzyme activity: Amylase from plant tissue & saliva.
10. Determination of K_m and V_{max} of enzyme catalysed reaction.

Introduction to Practical Biochemistry: Plummer, Tata McGraw Hill.

3rd semester

MCYC301 ORGANOMETALLIC CHEMISTRY

MODULE-I **(14Hours)**

Making sense of organomettalic complexes, the 18- e^- rule and its limitation. Electron counting in reactions. Oxidation state, co-ordination number and geometry. Effect of complexationwith different metals (4d and 5d).

Alkyls and hydrides: alkyls and aryls(metal alkyls stabilized carbanion, β-elimination,stable alkyls, agostic alkyls, reductive elimination, preparation of metal allyls).metal hydrides: characterization, synthesis, reactions, bridging hydrides.

MODULE-II **(12 Hours)**

Pi complexes, synthesis, bonding. Properties and application of alkenes and alkynes, allyls, diene, cyclopentane,dienyl,arenes.

Oxidative addition and reductive elimination: concerted addition, SN^2 pathways. Radical mechanisms, ionic mechanism.
Insertion and Elimination: CO insertion, alkene insertion, outer sphere insertion, α, β, δ, γ elimination.

MODULE-III **(14Hours)**

Addition and abstraction: Nucleophilic addition toCO, Nucleoplic addition to polynes and polyenyls ,nucleophilic abstraction in hydrides, acyls, electrophilic addition and abstraction, single electron transfer and radical reactions.

Transition metal organometallic in organic sysnthesis: Alkene isomerisation, hydrogenation, hydroformylation, hydrocyanation, hydroboration, coupling reaction.

Books:

1. The Organometallic Chemistry of the Transition Metals **,** by Robert H. Crabtree, Wiley 2014
2. Organotransition Metal Chemistry: From Bonding to Catalysis by John F. Hartwig, University Science Books, 2009
3. Organotransition Metal Chemistry, Anthony F.Hill, Royal Society of Chemistry,
1. Tutorial Chemistry Text, 2002. Chapters 1 to 7.
4. Organometallics: A concise Introduction, Ch.Elshebroicn and A Salzer, VCH, 2006.
5. Organotransition Metal Chemistry: Applications to Organic Synthesis, S.G.Davies, Pergamon 1982.

MCYC302CHEMISTRY OF DRUG DESIGN

Module I

Medicinal plant: Historical aspects . **(12Hours)**

Biopharmaceutical Properties of Drug Substances : Biological membrane, passive diffusion, physiochemical properties Vs Drug absorption, lipid solubility, drug dissolution Vs Drug absorption, Acid-Base properties, Drug receptor Interaction.

Metabolic Changes of Drugs and Related Organic compounds : Sites of Drug Biotransformation, role of Cytochrome P-450 Monooxygenase in Oxidative Biotransformation, Oxidative Reactions, Reductive Reactions, Hydrolytic Reactions, Phase-II or Conjugation Reactions, Factors affecting Drug Metabolism.

Module II **(14Hours)**

Structural Features and Pharmacological Activity : Optical and Geometrical isomerism and pharmacologic activity, conformational isomerism and pharmacologic activity, effects of conformational isomerism on biological activity of Drugs Bioisosterism.

Theoretical Aspects of Drug Design : Molecular modeling, Rational drug design, Principles of Combinatorial Chemistry, QSAR.

Anti-Materials : Etiology, Quinolines and Analogy, DiaminoPyrimidines, Biguanides.

Anti-Neoplastic Drugs: Alkylating agents, Antimetabolites, Antibiotics, Plant Products, Immuno Therapy.

Module III **(14Hours)**

Central Nervous System Depressants :Axiolytic, Sedatives and Hypnotic agents, Antipsychotics, Anticonvulsant and Antiepileptic Drugs.

Central Nervous System Stimulants : Analeptic, Methylxanthines, Antidepressant Compounds, Psychadetics.

Drugs Affecting Sugar Metabolism: Diabetes Mellitus - The disease, Insulin, mechanism of action, Oral Antidiabetic Agents- Biguanides,sulfonylureas, hazards and side effects.

Anti-viral Drugs : Adamantine hydrochloride, Interferon, Zidovudine agents interfering with Viral Nucleic Acid Replication -Acyclovir, Idoxuridine, Vidarbine.

Books:

1. The Organic Chemistry of Drug Design and Drug Action – by Richard B. Silverman &, Mark W. Holladay = 3rd edition- 2014- Academic Press
2. MedicinalChemistry:ABiochemicalApproach, Thomas Nogrady
3. Drug Discovery Strategies and Methods by AlexandrosMakriyannis, Diane Biegel, 2003, CRC press
4. Textbook of Drug Design and Discovery, -edited by Tommy Liljefors, PovlKrogsgaard-Larsen, Ulf Madsen -Third Edition-– CRC press
5. Drug Design Strategies = David J Livingstone , Andrew M Davis –RSC publishing- 2011
6. Drug Design by Klebe Gerhard by Springer
7. PrinciplesofMedicinalChemistry,William O.Foye
8. The PharmacologicalBasisofTherapeutics:GoodmanandGilman
9. IntroductiontoDrug Metabolism,G.GordonGibsonandPaulSket

MCYF301 ENVIRONMENTAL CHEMISTRY

Module – I **(12 Hours)**

Ecological Concepts: Biotic components, Ecosystem Process: Energy, Food Chain, Water cycle, Oxygen cycle, Nitrogen cycle, carbon cycle, Environmental gradients, Tolerance levels of environment factor, EU, US and Indian Environmental Law. Chemistry in Environmental Engineering: Atmospheric chemistry, Soil chemistry. Noise pollution- Noise standards, measurement and control. Water Treatment: water quality standards and parameters, Ground water. Water treatment processes, Pre-treatment of water, Conventional process, Advancedoxidation process.

Module – II **(14Hours)**

(a)Waste Water Treatment: COD and BOD of Waste water treatment process, pretreatment, primary and secondary treatment of waste water, Activated sludge treatment: Anaerobic digestion, Reactor configurations and methane production.

(b)Air Pollution : Air pollution and pollutants, criteria of pollutants, Acid deposition, Global climate change –greenhouse gases, air pollution meteorology, Atmospheric dispersion. Industrial Air Emission Control. Flue gas desulphurization, NOx removal, Fugitive emissions.

(c) Solid waste, Hazardous waste management, Solid Waste Management, Source classification and composition of MSW: Separation, storage and transportation, Reuse and recycling, zero waste management, Hazardous Waste Management, Hazardous waste and their generation, Transportation and treatment: Incinerators,super critical liquids, Inorganic waste treatment. E.I.A., Environmental auditing,

Module – III **(14Hours)**

Occupational Safety and Health Acts, Safety procedures, Type of Accidents, Chemical and Heat Burns, Prevention of Accidents involving Hazardous substances, Human error and Hazard Analysis. Hazard Control Measures in integrated steel industry, Petroleum Refinery, L.P.G. Bottling, Pharmaceutical industry. Fire Prevention – Detection, Extinguishing Fire, Electrical Safety, Product Safety. Safety Management- Safety Handling and Storage of Hazardous Materials, Corrosive Substances, Gas Cylinders, Hydro Carbons and Wastes. Personal Protective Equipments.

Text Book

1. Environmental Engineering Irwin/ McGraw Hill International Edition, 1997, G. Kiely,
2. Industrial Safety Management, L. M. Deshmukh, Tata McGraw Hill Publication.

Reference Books

1. Chemistry for Environmental Engineering and Science, Clair N. Sawyer, Perry L. Mc Carty and Gene F. Parkin, 5th edition, Mc GrawHill
2. Environmental Engineering by Arcadio P. Sincero&Gergoria A. Sincero PHI Publication
3. Principles of Environmental Engineering and Science, M. L. Davis and S. J. Masen, McGraw Hill International Edition, 2004
4. Environmental Science, Curringham&Saigo, TMH,
5. An Introduction to Environmental Engineering and Science by Gilbert M. Masters & Wendell P. Ela - PHI Publication.
6. Industrial Safety Management and Technology, Colling. D A – Prentice Hall, New Delhi.

MCYF302 CHEMICALSYNTHETIC STRATEGYOFADVANCED MATERIALS & NANO MATERIALS

Module-1: (14 Hours)

Materials and their classification:Matter, materials science, broad classification of materials, -metal and alloys, polymers and elastomers, ceramics and refractories, semiconductor and electronic materials, super metal and super conductors, materials for nuclear technology and for aero-space technology, magnetic materials, dielectric materials, optical and opto-electronic materials, bio-medical materials, thermo- electrical materials, structural and construction engineering materials, special and nano materials, SMART materials.

General Strategies for preparation and production of materials: Wet chemical processes, the sol-gel route, precursor synthesis, carbo-thermic and thermo- chemical treatments, hydrothermal, pyrochemical, metallurgical and chemical routes, heat treatment methods, surface deposition and film formation methods, special fabrication and processing techniques.

Elementary ideas on basic properties of important materials (overview only): Mechanical properties and impact properties, brittle, malleable and ductile properties, crystalline, poly crystalline materials. Phase rule and phase diagram its applications.

Overview of material characterization:x- ray diffraction for internal structure, electron-microscopy for surface property.

Module-2: Dielectric and Magnetic Materials. (12 Hours)

Dielectric materials:Electrical dipole moment, dielectrics, dielectric constants and polarization, microscopic displacement, temperature and frequency dependence of dielectric constant, dielectric break down. Synthetic strategies for preparation of dielectric materials. Ferro electrics. Piezoelectric. Pyroelectrics. Application of dielectric materics.Magnetic materials:Concept/ origin of magnetism, dimagnetism, par magnetism, ferromagnetism,hysteresis- soft and hard magnets. Synthetic strategies. Ferrites, ortho-ferrites and plumba ferrites. Applications of magnetic material, magnetic bubbles.

Module-III: Semi-Conductor and Electronic Materials. (14 Hours)

Semi conductor and electronic materials:Band concept for insulator, conductor and semi -conductor(elementary), intrinsic and extrinsic semi-conductor, conductivity, n- and p- type semiconductor, carrier and hole mobility and concentration Fermi level, density of electrons in the conduction band and density of holes invalence band, concentration of electrons in the CB of n- type and holes in VB of p-type semiconductor. Hall effect- hall voltage and Hall coefficient and application. Fabrication and processing of semiconductors. Film formation and surface coating techniques. Application of semiconductors. Film formation and surface coating techniques. Applications of semi conductors. Preparation of single crystals. Microelectronic circuits.

Composites:Micro and macro composites, fibre -reinforced composites (FRPs), matrix based composites. Polymer- matrix composites (PMCs), metal- matrix composite (MMCs), ceramic- matrix composites (CMCs) as in construction materials, carbon- carbon composites (CCCs), hybrid composites. Uses of composites.

RecommendedBooks:

1. Magnetic and Dielectric Properties of Materials: Basics, Theories and Experiments – by Mohammad Mahbubur Rahman, 2012
2. Semiconductor Material and Device Characterization , by Dieter K. Schroder, Springer, 3rd edition 2006.
3. Introduction to Semiconductor Materials and Devices by M.S.Tyagi , John Wiley & Sons, 2008
4. The Materials Science of Semiconductors by AngusRockett Springer, 2008

5. ChemicalProcessingofAdvancedMaterials:L.L.HenchandJ.K.West(eds),JohnWileyNew York 1992.
6. P.Hagnmuller(ed):PreparativeMethodsinSolidStateChemistry,AcademicPress,NewYork,1972.
7. Sol-GelScience,C.J.Brinker&G.W.Scherer, AcademicPress, 1980. Non-OxideTechnical&Engg.Ceramics,Ed.StuartHampshire,ElsevierAppliedSciencePub.Ltd. 1986.
8. UltrastructureProcessingofCeramics,glassesandComposited,Ed.L.L.Hench,D.R.Ulrich, JohnWiley,NewYork1984.

MCYF 303 COMPUTER PROGRAMMING FOR CHEMISTRY

Module – I [12 Hours]
Algorithm, flowchart, Structured Programming Approach, structure of C program (header files, C pre-processor, standard library functions, etc.),identifiers, basic data types and sizes, Constants, variables, arithmetic, relational and logical operators, increment and decrement operators, conditional operator, bit-wise operators, assignment operators, expressions, type conversions, conditional expressions, precedence and order of evaluation. Input-output statements, statements and blocks, if and switch statements, loops:-while, do-while and for statements, break, continue, goto, programming examples.

Module – II [12 Hours]
Designing structured programs: - Functions, parameter passing, storage classes- extern, auto, register, static, scope rules, user defined functions, recursive functions. Arrays- concepts, declaration, definition, accessing elements, and functions, two-dimensional and multi-dimensional arrays, applications of arrays. pointers- concepts, initialization of pointer variables, pointers and function arguments, address arithmetic, Character pointers and functions, pointers to pointers, pointers and multidimensional arrays, dynamic memory management functions, command line arguments,

Module – III [12 Hours]

Derived types- structures- declaration, definition and initialization of structures, accessing structures, nested structures, arrays of structures, structures and functions, pointers to structures, self referential structures, unions, typedef, bit fields, C program examples. Input and output – concept of a file, text files and binary files, streams, standard I/O, Formatted I/O, file I/O operations, error handling, C program examples.

Applications tochemistry : statistical thermodynamics, chemical kinetics, Curve fitting, GaussianandLorentziandeconvolution

Useofsoftwarepackagessuchasvisualization,semi-empiricalmethods.

Text Books:

1. Balagurusamy : “C Programming” Tata McGraw-Hill
2. P. Dey& M. Ghosh, “Computer Fundamental & Programming in C”- Oxford University Press
3. Deitel -“C How to programme” PHI publication/ Pearson Publication
4. GausssianSofetware

Reference Books:

1. Y. Kanitkar – “Let us C” BPB Publisher
2. H. Schildt – “C the complete Reference” McGraw-Hill
3. Schaum Series- “C Programming” - Gotterfried
4. MichaelBoillot, UnderstandingFortran77,wess-publishingcompany,New York(1987).
5 Fortran95/2003forscientistsandengineers,S.J.Chapman,McGrawHill2008).
6. S.C.ChapraandR.P.Canale,NumericalMethodsforEngineers,TataMcGrawHill,NewDelhi(2003).

MCYC 350 ADVANCED PHYSICAL LAB

1. Determination of CMC of surfactants by different methods.
2. Adsorption isotherm studies
3. Kinetic studies of ester hydrolysis
4. pKs determination of tribasic acid by pH titration method
5. Iodination of acetone by spectrophotometric method
6. Fluorometry studies of pyrine emission
7. Study of fast reactions by Stopped flow Spectrophotometry.

MCYF351 ENVIRONMENTAL CHEMISTRY LAB

A. Water Quality Analysis

1. Determination of pH
2. Determination of turbidity.
3. Determination of alkalinity and acidity.
4. Optimum dose of coagulants by jar test.
5. Total Hardness.
6. Total solids and suspended solids.
7. Residual chlorine.
8. Chlorides.
9. Chemical Oxygen Demand.
10. Biochemical Oxygen Demand.
11. Dissolved Oxygen.

MCYF 352 – COMPUTER PROGRAMMING LAB. (0-0-3)

(Minimum 10 programs to be done covering 8 Experiments)
Experiment No. 1

a) Write a C program to find the sum of individual digits of a positive integer.
b) A Fibonacci sequence is defined as follows: the first and second terms in the sequence are 0 and 1. Subsequent terms are found by adding the preceding two terms in the sequence. Write a C program to generate the first n terms of the sequence.
c) Write a C program to generate all the prime numbers between 1 and n, where n is a value supplied by the user.

Experiment No. 2
a) Write a C program to calculate the following Sum:
Sum=1-x
b) Write a C program to find the roots of a quadratic equation.
Experiment No. 3
a) Write C programs that use both recursive and non-recursive functions
i) To find the factorial of a given integer.
ii) To find the GCD (greatest common divisor) of two given integers.
iii) To solve Towers of Hanoi problem.
Experiment No. 4
a) Write a C program to find both the larges and smallest number in a list of integers.
b) Write a C program that uses functions to perform the following:
i) Addition of Two Matrices
ii) Multiplication of Two Matrices
Experiment No. 5
a) Write a C program that uses functions to perform the following operations:
i) To insert a sub-string in to given main string from a given position.
ii) To delete n Characters from a given position in a given string.
b) Write a C program to determine if the given string is a palindrome or not
Experiment No. 6
a) Write a C program to construct a pyramid of numbers.
b) Write a C program to count the lines, words and characters in a given text.
Experiment No.7
a) Write a C program that uses functions to perform the following operations:
i) Reading a complex number
ii) Writing a complex number
iii) Addition of two complex numbers
iv) Multiplication of two complex numbers
(Note: represent complex number using a structure.) 21
Experiment No. 8
a) Write a C program which copies one file to another.
b) Write a C program to reverse the first n characters in a file.
(Note: The file name and n are specified on the command line.)

4th Semester

MCYC 401 APPLICATION OF ADVANCED INSTRUMENTAL METHODS (3-0-0)

Module I (12 hours)

Differential Scanning calorimetry (DSC) : principle, measurements, interpretation of data, oscillatory temperature profile, fast scanning DSC and its application to polymers, pharmaceuticals, water based solutions and effect of moisture.

Thermogravimetric Analysis; Principle, measurements, interpretation of of TGA curves, quantitative evaluation of thermal analysis data, application to thermoplastic resins and rubbers,

Thermal mechanical analysis and interpretation of data its applications.

Module II (14 hours)

Characterization of Organic Compounds and their structures by using UV-Visible, IR, NMR and ESR spectral data.

Module III **(14 hours)**

Chromatography: GC, TLC, SFC, HPLC. Basic concepts and controls of separation, columns selection and equipments, detection. Reversed-phase, ion-pair and ion-exchange chromatography and its application to neutral samples, gradient elution, qualitative and quantitative analysis. Molecular structure and conformation of biomolecules, separation of biomolecules, proteins, peptides, polymers, enantiomers.

Recommended Books

1. Principle and Applications of Thermal Analysis by Paul Gabbott, John Wiley & Sons (Blackwell Publshing), 2009.
2. Pretsch**,** Ernö, Bühlmann**,** Philippe, Badertscher**,** Martin, Structure Determination of Organic Compounds, 4th edition, Springer, 2009.
3. Lloyd R. Snyder (Author), Joseph J. Kirkland (Author)Introduction to Modern Liquid Chromatography Hardcover, 3rdedn., Wiley,2009
4. Ian A. Fowlis, Gas Chromatography, 2nd edition, John Wiley & Sons, Ltd, 1995.
5. D. Bliesner , Validating Chromatographic Methods: A Practical Guide , John Wiley & Sons, 2006
6. Jeffrey Simpson, Organic Structure Determination Using 2-D NMR Spectroscopy, 2012, Academic Press.

MCYC 402 POLYMER CHEMISTRY (3-0-0)

Module I (12 hours)

Fundamental concepts - functionality - principle of polymerisation - addition, condensation polymerisation - ring opening polymerisation - classification - production from coal tar and petrochemicals - Techniques of polymerisation - gas polymerisation, - bulk, solution, suspension and emulsion - melt condensation.

Mechanism of polymerisation and general characteristics - free radical - cationic, anionic and coordinationpolymerisation (Ziegler-Natta catalyst) autoacceleration - Kinetic chain length - degree of polymerisation kinetics of polymerisation (Detailed study) - copolymerisation.

Module II (14 hours)

Polymer characterisation - molecular weight, MWD - Mn, Mw, Mv and Mz - end group analysis - viscometry - osmometry - Light scattering - spectral analysis-Thermal properties – Electrical properties, Mechanical and dynamic properties - polymer degradation. Phase transitions of polymers, crystallization and glass transition, mechanism of glass transition , methods of determining Tg.

Module III (12 hours)

Studies of individual polymers - plastics - polyolefins, polystyrenes, acrylics, polyesters, polyamides, cellulose, polyurethanes, Inorganic polymers, FIR plastics - GRplastics. alkyd resins, epoxy resins - phenolics - Melamine resins - compounding of plastics - rubber - elastomer - vulcanisation, compression mouldings - injection mouldings - lamination . Biopolymers - Biomaterials - medicinal applications of polymers - High temperature and fire resistant polymers. Polymer concrete - polymer impregnated concrete - conducting polymers - polymeric reagents.

Text books

1. P.J. Flory, 'Principles of Polymer Chemistry' , Cornell Press,(Recent Edition).
2. Jr. Billmeyer, ' Test Book of Polymer Science', Fred, W. John Wiley & Sons, New York, l984.
3. Dan Campbell, Richard A. Pethrick, Jim R. White, Polymer Characterization: Physical Techniques, 2nd Edition, CRC Press, 2012.

References

1. F. Rodrigues, 'Principles of Polymer Systems', M. Elpaw Hill Book Company, 2nd Edn., l982.
2. K.J.Saunders, , 'Organic Polymer Chemistry', Chapman & Hall, London, l973.

3. Sabu Thomas&Dominique Durand, Handbook of Biopolymer-Based Materials: From Blends and Composites to Gels and Complex Networks , Wiley – VCH, 2013

MCYC 403 SOLID STATE CHEMISTRY (3-0-0)

Module I

Chemicalcrystallography (14 hours)

Introduction, Space lattice, Crystal point groups, space group (working knowledge), Stereographic projections,Packinginsolids,Crystalstructuresofrepresentativesystems, SilicatesandZeolites,Cements,Glasses, Quasicrystals,Nanostructures.

BondinginsolidsandCrystal energetics

Crystalclassifications,Madelungconstant andLatticeenergy.

Module II (12 hours)

ElectronicpropertiesandBand theoryofsolids

Freeelectronmodel,Metals,semiconductorsandinsulators, dopedsemiconductors Solidstate ionics.

Defects,Nonstoichiometry andDiffusion

Pointdefects,Dislocations,Extendeddefects,Clustersandaggregates,Colorcentres,Non-stoichiometryofcompounds,Diffusionmechanisms,Fick'slaw,Kirkenalleffect.

Phasetransitions

Criticalphenomena,varietyofphasetransitions(Ordered-disorder,Martensite-austenite, Spinoidaldecompositions etc), Liquid crystals, Structure-property relations (magnetic, electrical,superconductivity,opticalandthermal).

Module III

Preparative and characterization techniques (14 hours)

Powder synthesis by conventional and modern chemical methods, Reactivity of solids, Decompositionmechanisms,Powderprocessing(sinteringanddiffusionprocesses),Tailoring ofsolids, Specialmethodsforsinglecrystalgrowthandthin films depositions.

Characterizationtechniques(workingknowledge)for solids

X-raydiffraction,Electronmicroscopy(SEM,TEM,AFM), Spectroscopic techniques (Mossbauer, IR, UV-VIS) and Physical property measurementtechniques(Magneticmoments-VSM/SQUID,Electricalresistivity–Two/Four probemethods andthermalconductivity,Opticalbandgap,XPS, XAS).

Recommendedbooks:

1. A.R.West,SolidStatechemistryandits applications, 2nd edition, JohnWiley& Sons,.
2. L.Smart andE.Moore,SolidState chemistry:AnIntroduction, 4th edition, ChapmanandHall.
3. A.K.CheethamandP.Day,Solidstatechemistrycompounds,ClarendonPress, Oxford1992.
4. C. N. R. Rao andJ. Gopalkrishanan, Newdirections in solid state chemistry, CambridgeUniv.Press 1997.
5. S.E. Dann, Reactions and Characterization of Solids, , ISBN 0-471-22481-2
6. A.R. West , Basic Solid State Chemistry, Wiley, 3rd edition, 2012
7. Christopher Hammondhy, The Basics of Crystallography and Diffraction (International Union of Crystallography Texts on Crystallograp), Wiley 2009

MCYF 404 NUCLEAR CHEMISTRY

Module I **(12 hours)**

General Aspects of Nuclear Chemistry: Discovery- Types of decay-Decay kinetics: Decay constant, half-life period, mean life Parent daughter decay-growth relationships-Secular and transient equilibrium-Units of radioactivity- Alpha, beta and gamma decay: Theory of decay, energies and properties-Artificial radioactivity- Detectors: Ionization chamber, electron pulse counters, scintillation detectors, semiconductor, detectors, thermo luminescence detectors and neutron detectors. Bethe notation-Types of nuclear reactions: The compound nucleus theory-Reaction crosssection- Transmutation reactions, elastic and inelastic scattering, spallation, fragmentation, stripping and pick-up, fission, fusion, photonuclear reactions, Thermonuclear reactions.

Module II **(10 hours)**

Nuclear Disintegration and Reactors:The fission energy – Reproduction factor - Classification of reactors- Based on Moderators, Coolent, Phase of Fuel and Generation -Principle of Thermal nuclear Reactors: The four factor formula - Reactor power – Critical size of a thermal reactor – Excess reactivity and control - Breeder reactor - Reprocessing of spent fuels - Nuclear waste management – Safety culture – Active and passive safety, containment building, nuclear criticality safety, ionizing radiation protection – enforcement agencies.

Module III **(14 hours)**

Radiation chemistry – Passage of radiation through matter – Units for measuring radiation absorption – Radiation dosimetry – Radialysis of water – Free radicals in Water Radiaolysis – Chemical dosimetry: Radiolysis of Fricke Dosimeter Solution – Radiation-induced colourcentres in crystals – Effects of radiation with matter: Radiolysis of inorganic gases, organic gases, organic compounds, solids, and polymers- Annealing of radiation damage.

Application of radioisotopes: probing by isotopes, reactions involved in the preparation of radioisotopes, The Szilard-Chalmer's Reaction – Radichemical principles in the use of Tracers – Applications of radioisotopes as tracers- Chemical investigations, analytical applications, agricultural and industrial applications -Neutron Activation Analysis – Carbon and Rock Dating – Use of nuclear reactions- Radioisotopes as source of electricity – Nuclear medicines.

Text Books

1. Walter Loveland, David Morrissey, Glenn Seaborg. Modern Nuclear Chemistry, Wiley-Interscience, Hoboken, NJ, 2006
2. Arnikar, H. J., 'Essentials of Nuclear Chemistry', 4th Edn., New Age International Publishers Ltd., New Delhi, 1995.

References

1. K. H. Lieser, Nuclear and Radiochemistry, 2nd revised ed., Wiley-VCH, Berlin, 2001.
2. G. Choppin, J. O Liljenzin and J. Rydberg. Radiochemistry and Nuclear Chemistry. 3rd ed. Butterworth-Heinemann, Oxford, 2002.
3. Walter D. Loveland, David J. Morrissey.Modern Nuclear Chemistry ,wiley 2005.

MCYF 405 SYNTHESIS OF FINE CHEMICALS

Module I (14 hours)

Microwave-assisted synthesis of bioactive heterocyles in aqueous media, reactions on the solid surfaces (zeolites, clay, Al_2O_3, SiO_2), high pressure activation methods, mechanochemical mixing and microwave irradiation. Biocatalysis, Biosynthesis, cell culture technology.

Module II **(12 hours)**

Assymetric Synthesis: prochirality, achiral and chiral molecules and their properties, enantioselective and diastereoselective synthesis and methods of monitoring, classification, chiral boron reagents, chiral catalyst mediated asymmetric reactions of enzymes, chiral organometallic catalysed asymmetric reactions, asymmetric Diels-Alder reactions.

Module III **(14 hours)**cardiovascular drugs, such as Alapril (lisinopril), Captoril (captopril), .antiulcerants (cimetidine. .

artificial sweetener Aspartame (N-L-α-Aspartyl-L-phenylalanine 1-methyl ester) , riboflavin (B2), and thiamine (B1)

References

1. Eco-friendly Synthesis of Fine Chemicals, Edited by Roberto Ballini from RSC Green Chemistry Series, edited by James H. Clark and George A. Kraus, Royal Society of Chemistry, 2009
2. Aqueous Microwave Assisted Chemistry: Synthesis and catalysis, ed. V. Polshettiwar and R. S. Verma, from RSC Green Chemistry Series, Royal Society of Chemistry, 2010

3. G. L. David Krupadanam, Fundamentals of Assymetric Synthesis, Universities Press, 2013

MCYF 406 SUPRAMOLECULAR CHEMISTRY

Module I (12 hours)

Introduction-
themeaningofsupramolecularchemistry,phenomenonofmolecularrecognition andtheir quantification

Building blocks of supramolecularchemistry- acyclic receptors for neutral and charged guests, macrocyclesand crown ethers, macrobicyclesand cryptands, macropolycycles, cucurbiturilsandcyclodextrins

Module II(15 hours)

Sensors andinformation processing, electro-optic phenomena, molecular machines

Amphiphilicmoleculesandtheiraggregation,Langmuir-
Blodgettry,molecularrecognitionat theair-waterinterface.

Module III (13 hours)

Discreteandpolymericmetal-organichybridmaterials-
guestinclusion,catalysisandother applications.

Books

1. SupramolecularChemistry:ConceptsandPerspectives,J.-M.Lehn,VCH, Weinheim, 1995
2. PrinciplesandMethodsinSupramolecularChemistry,H.J.SchneiderandA.Yatsim irsky, Wiley, NewYork,2000
3. SupramolecularChemistry,J.W.Steedand J.L.Atwood,JohnWiley&Sons, Chichester,
   2009
4. Ariga, Katsuhiko&Kunitake, Toyoki, Supramolecular Chemistry - Fundamentals and Applications , 2006, Iwanami Shoten Publishers, Tokyo

MCYF 407 CHEMISTRY OF NATURALPRODUCTS

Module I (14 hours)

Introduction to natural products: Isolation and structure elucidation of terpenes, alkaloids, flavonoids, xanthones. Structural elucidation of strychinine, tylophorine, morphine, abietic acid.

Module II (12 hours)

Biosyntheticaspects andSynthesisofselectednaturalproductsofbiologicalandstructural importance:benzylisoquinoline alkaloids, colchicines, quinine, terpenes (mon, di and tri), isoflavones, anthraquinones.

Module III (14 hours)

Total Synthesis: Taxol, erythronolide B, penicillin V, Prostaglandins F2-alpha and E2.

Books:

1. K.C.Nicolaou, "Classics inTotalSynthesis" VolsI-III,Wiley-VCH, 1996;2003;2011
2. T.HudlickyandJ.W.Reed, "The way ofsynthesis",Wiley-VCH, 2007
3. E.J.Corey andX-M.Cheng,"Thelogic ofchemicalsynthesis, John-Wiley& Sons,NewYork, 1989.
4. D.H.R.Barton,K.Nakanishi,O.Meth-Cohn,"Comprehensivenaturalproductschemistry" Vols1-9, Elsevier,1999.
5. N. R. Krishnamurty, Chemistry of Natural Products, University Press, 2nd edition 2010.

MCYF 408 FRONTIERSINORGANICCHEMISTRY

Module I (10hours) GreenChemi

Module II (14 hours)

Organic Magnets: theoretical methodologies, molecular orbital description of magnetic organic systems, strongly coupled magnetic molecules, photomagnetic effects.
Organic LED: generation of excited states and its decay pathways, optical properties of organic LEDs.
Organic Conductors: basic physical concepts, molecular design, chemical synthesis, optical properties.

Module III (14 hours)

Combinatorial chemistry: Resins, protecting groups, solid-phase synthetic strategies, synthesis of peptides, synthesis of some novel biologically important N-heterocyclic building blocks using amino acids, techniques for preparation of combinatorial libraries.

Books:

1. T.K.Lidhorst,"Essentiallofcarbohydratechemistryandbiochemistry,Wiley-VCH,2006
2. Farges, Organic Conductors: Fundamentals and Applications (Applied Physics), CRC press, 1994
3. Sambhu N Datta **&**FrancescIllas **,** Theoretical and Computational Aspects of Magnetic Organic Molecules, 2014, world scientific.
4. Jan Kalinowski, Organic Light-Emitting Diodes: Principles, Characteristics &Pocesses (Optical Science and Engineering) Hardcover – CRC press, 2004
5. J.Tsuji,"Transitionmetalreagentsandcatalystinnovationsin organicsynthesis" John-Wiley-&Sons, Ltd,NewYork,2000
6. W. Bannwarth, B. Hinzen, Combinatorial Chemistry - From Theory to Aplication
7. Wiley-VCH, 2nd edition, 2006.
8. Michael Pirrung, Molecular Diversity and Combinatorial Chemistry, Elsevier, 204.
9. Review articles on Combinatorial chemistry

MCYF 409 FRONTIERS IN INORGANIC CHEMISTRY

Module I (12 hours)

Size, Shape, facet, selective catalysis covering photosynthesis. Metal storage and transportation, pathways for catalysis of Zn and Cu enzymes, Water splitting and its importance to non-conventional energy resources

Module II (14 hours)

Reductivecleavageofdioxygenbond, biological dioxygen carriers, dioxygen reactions, cytochrome c oxidase, cytochrome p-450, catalase, peroxidase, Cu-Zn superoxide dismutase. Novelorganictransformations by metalloenzymes of Fe and Cu.

Module III (14 hours)

Metal Sulphide proteins: Fe and Cu. Structural and the Enzymatic catalysis of hydrolysis and condensations reactions of Zn. Enzymatic reactions, Important catalytic activities of Al, Pd, and Ti.

Books

1. BioinorganicChemistry,I.Bertini,H.B.Gray,S.J.LippardandJ.S.Valentine,University ScienceBooks, MillValley,2006.

2. Wolfgang Kaim, Brigitte Schwederski, Axel Klein, Bioinorganic Chemistry -- Inorganic Elements in the Chemistry of Life: An Introduction and Guide, 2nd Edition, wiley, 2013

MCYF 410 CHEMICAL REACTION DYNAMICS

Module I (12 hours)Introduction: Reviewofkinetic theoryofgases, collisions-atomic andmolecular.

Rate theories :Transitionstate theoryandRRKM theory,scattering phenomena-classicalandquantum.
Oscillatory Reactions: Theory with examples.

Module II (12 hours)
ReactiveCollisions: Potentialenergysurfaces,atom-diatomreactions,polyatomicreactions,state-selective, molecularbeams,reactionrates andcrosssections.

Module III (16 hours)
Dynamicsingasphase :Photodissociation,energytransfer,stereodynamics,chemistryinrealtimewithlasers, control.

Dynamicsincondensedphase :Solvation, diffusion, barrier crossing, Kramer-Grote-Hynes theory, Langevinequation, correlation functions.

RecommendedBooks

1.Levine, MolecularReactionDynamics,2005.
2.Henriksen&Hansen,TheoriesofMolecularReactionDynamics,2008.
3.Schinke,PhotodissociationDynamics,1993.
4.Manz&Wöste,FemtosecondChemistry,1995.
5.Nitzan,ChemicalDynamicsinCondensedPhases, 2006.

MCYF 411 ENZYME:REACTIONSMECHANISMAND KINETICS

Module I **(12 hours)**

Enzymekineticsofsingleandmultiplesubstratesystemsincluding Enzymeassaysa nd inhibition .

Module II **(12 hours)**

Cooperativityandmultienzymesystems.

Enzymestructureandidentificationofactive site residueslabelin,chemicalmodificationand mutagenesis.

Module III **(14 hours)**

EnzymeMechanisms–Methodsofstudy andmechanisms ofsome enzymeslike

Serineproteases,polymerases, ribonucleases,lysozymeandribonucleotidereductases (radicalenzyme).

Mechanismbasedenzymeinhibitionanddrugs–5-fluorouracilfor thymidylatesynthase.

Books:

1. 1.StructureandMechanisminProteinScience:AGuideto EnzymeCatalysis andProteinFolding by AllanFerhst
2. N.C.Price andE.Stevens,FundamentalsofEnzymology:TheCellandMolecularBiology ofCatalytic Proteins
3. I.H.Sigel,Enzyme Kinetics: Behavior and Analysis of Rapid Equilibrium and Steady-State Enzyme Systems, John Wiley & Sons, 1993.
4. Herbert M. Sauro, Enzyme Kinetics for Systems Biology, Wiley 2012
5. Athel Cornish-5. Bowden,Fundamentals of Enzyme Kinetics, Portland Press, 2004

MCYF 412 SINGLE MOLECULE SPECTROSCOPY

Module I **(12 hours)**

Molecular Dynamics of Single Molecules, Detection of Single Molecules and Single Molecule Processes. Single-Molecule Optical Spectroscopy and Imaging, Single Molecules as Optical Probes for Structure and Dynamics. Fluorescence Correlation Spectroscopy

Module II **(14 hours)**

Quantum Dots and Single Molecule Behaviour.- Development of Nanocrystal Molecules for Plasmon Rulers and Single Molecule Biological Imaging. Size-Minimized Quantum Dots for Molecular and Cellular Imaging.- Mapping Transcription Factors on Extended DNA: A Single Molecule Approach.- Molecular Motion of Contractile Elements and Polymer Formation.- Single Molecule Measurement, a Tool for Exploring the Dynamic Mechanism of Biomolecules.

Module III (14 hours)

Super-Resolution Fluorescence Imaging, Single-Pair FRET and Fluorescence QuenchingAlternating-Laser Excitation (ALEX),Single-Molecule Anisotropy and Polarization, In-vivo Single-Molecule Fluorescence

Books:

1. Graslund, Astrid, Rigler, Rudolf, Widengren, Jerker ,Single Molecule Spectroscopy in Chemistry, Physics and Biology, Springer Series in Chemical Physics, Vol. 96, 2010, XXII, 572p
2. AchillefsKapanidis,Mike Heilemann **,** Single-Molecule Fluorescence Spectroscopy of Molecular Machines, World Scientific, 2013.