Biju Patnaik University of Technology, Odisha
Two-Year (Semester System & Credit system) M. Sc. program
M.Sc. in Applied Chemistry

New Syllabus will be implemented from 2016-17 onwards.

PREAMBLE:

Duration – 2 year full-time course
Total No. of Semester – 4 (Two semesters per year)
Total No. of Theory Papers – 20 (each theory paper of 3 to 4 credit)
Total No. of Practical course – 8 (each practical paper of 2 to 3 credit)

No. of papers (theory) per semester – 4 / 5

No. of practical course per semester – 2 / 3

Grading System- 9 point credit system (2-10) with Maximum 10

DISTRIBUTION OF MARKS

Subject type	**Total points**	**Class tests**	**End semester examination**	**Pass points**
Theory papers (core, allied elective and free elective)	100	2 class tests of 15% points each	70 % points	25 out of 70 & 12 out of 30
Practical/Laboratory	100	Minimum 10 experiments @ 10 % points	-	50% points
Project	100	-	-	50 % points
Seminar	100	-	-	50 % points

Minimum Credit Requirement for Award of Degree: 100

ELGIBILITY FOE ADMISSION:

+3 Sc. , preferably Chemistry honors, passed out students

MEDIUM OF INSTRUCTION: English

STRUCTURE OF SYLLABUS

Semester - I

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC101	Inorganic Chemistry-I	3-1-0	4
Theory	MCYC102	Organic Chemistry-I	3-1-0	4
Theory	MCYC103	Physical Chemistry-I	3-0-0	3
Allied Elective	MCYE104	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	Organic Chemistry Laboratory	0-0-6	3
		Total	**30**	**24**

Semester - II

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC201	Inorganic Chemistry-II	3-1-0	4
Theory	MCYC202	Organic Chemistry-II	3-1-0	4
Theory	MCYC203	Physical Chemistry-II	3-0-0	3
Allied Elective	MCYE204	Spectroscopic Identification of Molecules	3-1-0	4
Free Elective	MCYF205	Chemical Biology	3-0-0	3
Practical	MCYC250	Inorganic Chemistry- II Laboratory	0-0-6	3
Practical	MCYC251	Physical Chemistry-I Laboratory	0-0-3	2
Practical	MCYF252	Computational Chemistry Laboratory	0-0-6	3
		Total	**33**	**26**

Semester - III

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC301	Analytical Techniques - I	3-0-0	3
Theory	MCYC302	Organic Chemistry-III	3-0-0	3
Free Elective	MCYF303	Environmental Chemistry	3-1-0	4
Free Elective	MCYF304	Materials Chemistry	3-0-0	3
Free Elective	MCYF305	Solid State Chemistry	3-0-0	3
Practical	MCYC350	Physical Chemistry –II Laboratory	0-0-6	3
Practical	MCYF351	Environmental Chemistry Laboratory	0-0-3	2
Practical	MCYF352	Chemical Biology Laboratory	0-0-3	2
	MCYC-314	Seminar	0-0-3	2
		Total		**25**

Semester - IV

Subject type	Subject code	Subject name	L-T-P	Credit
Theory	MCYC401	Analytical Techniques - II	3-0-0	3
Theory	MCYC402	Polymer Chemistry	3-1-0	4
Free Elective	-	Elective-I	3-1-0	4
Free Elective	-	Elective-II	3-1-0	4
	MCYC450	Project	0-0-15	10
		Total		25
				25

Choose one paper from each group of Elective-I and II

Group	**Elective - I**	**Elective - II**
Group-A	MCYF 403- Pharmaceutical Chemistry-I	MCYF 404- Pharmaceutical Chemistry-II
Group-B	MCYF 405- Synthesis and Characterization of Materials	MCYF 406- Advanced and Functional Materials
Group-C	MCYF 407- Chemistry of Natural Products	MCYF 408- Supramolecular Chemistry **or** MCYF 409- Nuclear Chemistry

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)

1st Semester

MCYC101 Inorganic Chemistry (3-1-0) 4 credits

Module I

Stereochemistry and Bonding in Main Group Compounds

VSEPR, Walsh diagrams, dπ-pπ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Metal - Ligand Bonding

Limitations of CFT, MOT: sigma bonding and energy level diagram in octahedral, tetrahedral and square planar complexes; pi-bonding and energy level diagram in octahedral complexes, angular overlap model.

Module II

Electronic Spectra of Coordination Compounds

Spectroscopic ground states, term symbols for d^n ions, Racah parameters, selection rules and intensities of bands, Orgel diagram, correlation and Tanaube-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent metal ions (d^1-d^6), divalent Mn, Co and Ni, $CoCl_4^{2-}$, calculation of Dq, B and β parameters, CT spectra.

Spectral properties of lanthanide and actinide metal complexes.

Module III

Metal-ligand Equilibria in Solution

Stability of metal complexes, Stepwise and overall stability constant, factors affecting the stability constant, determination of stability constants and their applications, compositions of metal complexes by Job's method..

Inorganic Reaction Mechanism

Reactivity of metal complexes, inert and labile complexes, factors affecting the reactivity of complexes, mechanisms of substitution (acid, base and anation) reactions of octahedral complexes, isotope effects, Berry's pseudo rotation, Swain-Scott equation, substitution reactions of square planar complexes, trans-effect – theories and applications in synthesis of metal complexes, Redox reactions: mechanism of one election transfer reaction (inner sphere and outer-sphere), Marcus theory for outer-sphere reactions.

Selected Text/Reference Books:

1. D. F. Shriver, P. W. Atkins, *Inorganic Chemistry,* 3rd Edn., Oxford University, Oxford, 1999.
2. N. N. Greenwood, A. Earnshaw, *Chemistry of the Elements,* Pergamon Press, 2nd Edn., 2002.
3. B. Douglas, D. McDaniel, and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, New York. 1993
4. D. Katakis, and G. Gordon, *Mechanism of Inorganic Reactions*, John Wiley & Sons: N. Y (1987).
5. J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, *Principles of Structure and Reactivity (1st impression)*, Pearson Education, 2006.
6. F. Basolo & R. G. Pearson, *Mechanism of Inorganic Reactions*, Wiley Eastern, 1967.
7. F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry,* 6th Edn, John Wiley, 1999.
8. R. G. Wilkins, *The Study of Kinetics and Mechanism of Reactions of Transition Metal Complexes,* Allyn & Bacon, Boston, 1974.
9. Robert B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems,* Oxford University Press, 1998.
10. A.K. Das and M. Das, *Fundamental Concept of Inorganic Chemistry,* Vol. 4 and 5, CBS Publisher & Distributor Pvt. Ltd., New Delhi, 2014.

MCYC 102 Organic Chemistry-I (3-1-0) **4 Credits**

Module I **(14 hours)**

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 π- 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, enantiotropic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis.

Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape.

Module II

(12 hours)

Reaction Mechanism (Structure, Reactivity and Rearrangements):

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

Types of mechanisms: S_N2, S_N1, mixed S_N1 and S_N2 and SET, S_E1.

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 concept and its application in organic synthesis.

Effect of structure on reactivity: resonance and field effects, steric effect.

Quantitative treatment, 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 nonclassical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements.

The S_N1 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 and regioselectivity.

Module III **(14 hours)**

Aromatic Electrophilic Substitution Reactions:

The arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, diazonium coupling, Vilsmer reaction, Gattermann-Koch reaction.

The SNAr, S_N1, 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, effects of solvents on reactivity.

Text Books:

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, 7th Edition, Wiley, 2013.
2. Advanced Organic Chemistry Part A: Structure and Mechanisms, Carey, Francis A., Sundberg, Richard J, Fifth Edition, Springer International Edition, 2007.

Reference Books:

1. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Sixth Edition, John Wiley & Sons, Inc., New York,1985.
2. Structure and mechanism in organic chemistry, von C. K. Ingold. Cornell Univ. Press, Ithaca. 1953
3. Organic Chemistry, R. T. Moririson and R. N. Boyd, Sixth Edtion, Prentice-Hall, 1992.
4. Modern Organic Reactions, H. O. House, Benjamin-Cummings Publishing Co.,Subs. of Addison Wesley Longman,US;2nd edn, 1972..
5. Principles of Organic Synthesis, R. O. C. Norman and J.M.Coxon, Third Edition, Blackie Academic and Professional, 1993.
6. Pericyclic Reactions: A Mechanistic Study.S. M. Mukherji Macmillan India Press, New Delhi, ,1979.
7. Reaction Mechanism in Organic Chemistry, S. M. Mukherjii and S. P. Singh, Third Edition Macmillan India Press, New Delhi, 1976.
8. Stereochemistry of Organic Compounds. D. Nasipuri,Third Edition, New Age International, 2014.
9. Stereochemistry of Organic Compounds. P.S.Kalsi, Eighth Edition, New Age International, 2015.
10. Organic Synthesis: Clayden J., Greeves N, Warren S, and Wouthers, Second Edition Oxford University Press, 2000.

MCYC103 Physical Chemistry-I (3-0-0) (3 credits)

Module I (10 hours)

Thermodynamics: A brief survey of laws of thermodynamics.

Standard States for Gases, Liquids and Solids and its Applications. Free Energies, Enthalpies and Entropies of Ions in Solutions. Activity and Mean Activity Coefficients of Electrolytes and their Determinations, Debye-Huckel Limiting Law. Thermodynamics of Mixing–Mixtures of Volatile Liquids– ideal and Real Solutions and Activities-Excess Functions. Thermodynamic Derivations of Phase Rule, Applications to two component (eutectic) and three component systems involving solids and liquids (Acetic Acid – Chloroform - Water, NaCl-Na_2SO_4-H_2O, NH_4NO_3-$(NH_4)_2SO_4$-H_2O.

Module II (8 hours)

Statistical Thermodynamics: The Boltzman equation, most probable configuration and concept of residual entropy. The Boltzman distribution formula.

The concept of partition function, Molecular partition functions: translational, rotational, vibrational and electronic partition functions. Characteristic temperatures, Translational partition function of a mono-atomic gas and derivation of ideal gas equation. Principle of equipartition of energy.

Module III (10 hours)

Electrochemistry-I: Debye Huckel-Onsager equation for the equivalent conductivity of electrolytes – experimental verification of the equation –conductivity at high field and at high frequency –conductivity of non aqueous solutions-effect of ion association on conductivity. The electrode-electrolyte interface-electrical double layer-electro capillary phenomena- Lippmann equation–the Helmholz–Perrin–Guoy-Chapmann and Stern models, Electrokinetic phenomena Tiselius method of separation of proteins - membrane potential.

Module IV (8 hours)

Electrochemistry-II: Elecrodics - Mechanism of electrode reactions-polarization and overpotential –The Butler volmer equation for one step and multistep electron transfer reaction– significance of equilibrium exchange current density and symmetry factor- significance of transfer coefficient-mechanism of the hydrogen evolution reaction and oxygen evolution reactions. Some electrochemical reactions of technological interest-corrosion and passivity of metals-construction and use of Pourbaix and Evans diagrams- methods of protection of metals from corrosion, Fuel cells - electro deposition.

Text Books

1. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, 1965.
2. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach,Viva Student Edition,2015.
3. R. J. Silbey, R. A. Alberty, M. G. Bawendi, Physical Chemistry, Wiley, 4th Edition, 2005.

References

1. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970.
2. P.W. Atkins, Physical Chemistry, 8th Edn., Oxford University Press, 1998.
3. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry, Shobanlal Nagin Chand Co, 1986.

MCYE104 Quantum Chemistry and Group Theory (3-1-0) (4 credits)

Module-I (12 hours)

Quantum Chemistry-I: Operators in Quantum mechanics: Linear, Hermitian and Angular Momentum operators, Eigenvalue problem.

Basic postulates of quantum mechanics. The Schrodinger equation, Particle in 1,2 and 3-dimensional boxes, degeneracy.

Module-II (8 hours)

Quantum Chemistry-II: Harmonic oscillator, Spherical Coordinates: Rigid rotator, Solution of the Schrodinger equation for Hydrogen like atoms, Significance of n, l and m quantum numbers. Linear Variation and Perturbation Methods. Multielectron atoms, spin quantum number, Ground and excited state of helium atom.

Module-III (10hours)

Quantum Chemistry-III: Hydrogen Molecule ion, Born-Oppenheimer approximation, LCAO-MO approximation, Hydrogen Molecule, Valence Bond and Molecular Orbital Theory. Homonuclear and heternuclear diatomic molecules (HF, CO, NO)

Module-IV (10 hours)

Group Theory: Symmetry Elements and Symmetry Operations, Point Groups, Representation of Groups, Reducible and Irreducible Representation; Character Tables, Applications of Great Orthogonality Theorem.

Text Books (Quantum Chemistry and Group Theory)

1. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach,Viva Student Edition,2015.
2. D. A. McQuarrie, Quantum Chemistry,Viva Student Edition,2015.
3. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishers,1988.
4. Cotton, F. A. Chemical Applications of Group Theory, 3rd Edn., John Wiley and Sons, 2003.

Reference Books

1. N. Levine, 'Quantum Chemistry', 4th Edn., Prentice Hall India, 2001.
2. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994.
3. Jack Simons, Introduction to Theoretical Chemistry, Cambridge University Press, 2003.
4. P. W. Atkins. Molecular Quantum Mechanics, Oxford University Press (1986).

MCYE105 Molecular Spectroscopy (3-0-0) (3 credits)

Module I (8 hours)

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.

Module II (8 hours)

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.

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.

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

Module III (8 hours)

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.

Module IV (10 hours)

NMR: General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift, Karplus curve, variation of coupling constant with dihedral angle.

Electron Spin Resonance: Electron spin and Magnetic moment , Resonance condition in ESR and significance of 'g' value . ESR spectra of organic free radicals , McConnel relation , applications of ESR.

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

Text Books (Molecular Spectroscopy)

1. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, Springer, 4th edn, 2004.
2. J. M. Hollas, Modern Spectroscopy, Wiley, 4th edn, 2003.

Reference Books

1. Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Weil, John A, J. R. Bolton, and Wertz, J. E, Wiley-Interscience, New York, (1994).
2. Basic One- and Two-Dimensional NMR Spectroscopy, H. Friebolin, VCH, 1991.
3. Bunker & Jensen, Molecular Symmetry & Spectroscopy, 1998.
4. Bernath, Spectra of Atoms and Molecules, 1995.

MCYC150 Inorganic Chemistry –I Laboratory (0-0-6) (3 credits)

I. Semi micro qualitative analysis of inorganic mixtures containing anions, common cations, less familiar element (W, Mo, Ce, Th, Zr, V and U), insoluble (sulphate, oxides, halide).

II. Preparation and quantitative analysis of complexes

- Cis-potassium diaquabis(oxalate)chromate(III) complex [analysis of oxalate and chromium]
- Hexamminecobalt(III)chloride [analysis of cobalt]
- hexamminenickel(II)chloride [analysis of nickel]
- Preparation of pentamminechloro cobalt(III)chloride.
- Chrome alum
- Copper(I) chloride
- Tris(thiourea) copper(I) complex
- Potassium tris-(oxalato)aluminate(III)
- Hexaaminecobalt(III) chloride
- Tetraaminecopper(II) sulphate.

III. Volumetric analysis

- Volumetric estimation of Ca and Mg in Dolomite solution.
- Volumetric estimation of Cu in Cu and Ni (German Silver).
- Volumetric estimation of Fe in Cu and Fe solution.
- Volumetric estimation of Zn in Cu and Zn solution.
- Volumetric estimation of Ni in Ni and Zn solution.

Selected Text/Reference Books:

1. G., Svehla, Vogel's Qualitative Inorganic Analysis, 6th Edn., Orient Longman New Delhi, l987.
2. V.V. Ramanujam, Inorganic Semi-micro Qualitative Analysis, 3rd Edn., National Publishing Company, Madras, l990.
3. J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny,Vogel's text book of Quantitative Chemical Analysis, 5th Edition, Longman Scientific and Technical (1999).
4. Hand-outs prepared for the laboratory experiments: collections from various literature sources
5. Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press, (India) Pvt. Ltd., 2002.
6. Roesky, H. W.; Möckel, K., Chemical Curiosities: spectacular experiments and inspired quotes, VCH, 1996.

1st Semester/ MCYC151 Organic Chemistry Practical (0-0-6) (3 Credits)

Qualitative Analysis

i. Identification of organic compounds, separation, purification and identification of compounds of binary mixture using TLC and column chromatography. Interpretation of IR spectra for functional group identification.
ii. Isolation of active natural products (caffeine, lycopene, etc.) from natural sources.
iii. Preparation of paracetamol, aspirin, and some dyes and indicators.
iv. Application of steam distillation in isolation of essential oil (clove) and perfume (rose).
v. Preparation of o-iodobenzoic acid from anthranilic acid, furoic acid from furfural.
vi. Thiamine catalysed benzoin condensation
vii. P reparation of benzil from benzoin.
viii. Estimation of phenol, aniline, ascorbic Acid.
ix. Estimation of glucose by Fehling's method & Bertrand's method.

Structure Drawing of various organic building blocks using chemdraw softwares

Text Books

1.Experiments and Techniques in Organic Chemistry, D. J. Pasto, C. R. Johnson & M. J. Miller, Printice Hall, 1992.

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',5th Edn. ELBS, London, l989.
5.Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.

2nd semester

MCYC201 Inorganic Chemistry-II (3-1-0) 4 credits

Module-I

Magnetic properties of coordination compounds

Types of magnetic behaviour, magnetic susceptibility and its determination by Gouy, Faraday and VSM method, Pascal's constants and constitutive corrections, paramagnetism, Curie-Weiss law, Van Vleck's equation (derivation exluded) and its applications, spin-orbit coupling, ferro- and anti-ferromagnetism coupling, super paramagnetism, high and low spin equilibria.
Anomalous magnetic moments, magnetic exchange coupling and spin crossover.
Magnetic properties of Lanthanide and Actinide metal complexes.

Module-II

Organometallic chemistry-I

Stability and 18 electron rules (covalent and ionic),
Alkyls/aryl and hydrides: alkyls and aryls (metal alkyls stabilized carbanion, β-elimination, stable alkyls, agostic alkyls, reductive elimination, preparation of metal allyls).
Metal hydrides: synthesis, characterization, reactions, bridging hydrides.
Pi-complexes: Synthesis, bonding, properties and applications of alkenes and alkynes, allyls, diene, cyclopentane, dienyl, arenes.
Introductory idea on transition metal-carbon multiple compounds: carbene and carbyne.

Module-III

Organometallic chemistry-II

Reactivity of organo-transition metal complexes: Coordinative unsaturation, substitution reactions (nucleophilic and electrophilic addition and abstraction), oxidative addition and reductive elimination, insertion reactions (insertion of CO, SO_2 and alkenes).
Catalysis by organo-transition metal complexes: Alkene isomerisation, hydrogenation and hydroformylation; Zeigler-Natta polymerization of ethylene, reduction of carbon monoxide by hydrogen (Fischer-Tropsch reaction).

Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as η^{2-} olefin, η^{3-} allyl and dienyl complexes.

Selected Text/Reference Books:

1. The Organometallic Chemistry of the Transition Metals**,** Robert H. Crabtree, Wiley, 2014.
2. Organotransition Metal Chemistry: From Bonding to Catalysis**,** John F. Hartwig, University Science Books, 2009.
3. Organotransition Metal Chemistry, Anthony F. Hill, Royal Society of Chemistry,
4. Tutorial Chemistry Text, 2002. Chapters 1 to 7.
5. Organometallics: A concise Introduction, Ch. Elshebroicn and A Salzer, VCH, 2006.
6. Organotransition Metal Chemistry: Applications to Organic Synthesis, S.G.Davies, Pergamon 1982.
7. A.K. Das and M. Das, *Fundamental Concept of Inorganic Chemistry,* Vol. 4 and 5, CBS Publisher & Distributor Pvt. Ltd., New Delhi, 2014.
8. *Organometallic Chemistry,* R.C. Mehrotra and A. Singh, New Age International Publishers, 2nd Edn, 2000.
9. Elements of Magnetochemistry, R.L. Dutta and A. Samal, S. Chand & Company Ltd., 1982.

MCYC202 Organic Chemistry-II **(3-1-0) 4 Credits**

Module 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.

Protecting Groups:

Principle of protection and deprotection of alcohol, amine, carbonyl and carboxyl groups and their application in organic synthesis.

Module II

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 annulation.

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

Module III

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 allyl systems.

Cycloadditons: Antarafacial and suprafcial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrengements: Suprafacial and antarafacial shifts of H, Sigmatroic shifts involving carbon carbon moieties, [3,3] and [5,5] Sigmatropic rearrangements, Claisen, Cope and aza-Cope rearrengements, fluxonal tautomerism, ene reaction.

Selected Text/Reference Books:

1. Designing Organic Synthesis, A Programmed Introduction to Synthon Approach, S. Warren, Second Edition, Wiley, 1978.
2. Organic Synthesis: Concepts, Methods and Starting Materials, J. Fuhrhop and G. Penzlin, VCH, Weinheim, Germany,2nd edn., 1993.
3. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press, 4th edn, 2004.
4. Modern Synthetic Reactions, H. O. House, W. A. Benjamin,2nd edn., 1972.
5. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, 7th Edition, Wiley, 2013.
5. Principles of Organic synthesis, R.O.C. Norman, J. M. Coxon, CRC Press, Third Edition, 1993.
6. Advanced Organic Chemistry Part B: Structure and Mechanism, Francis A. Carey, Richard J. Sundberg, Fifth Edition, Springer, 2008.
7. Organic Synthesis: The Disconnection Approach, S. Warren and P. Wyatt, Wiley India Pvt.Ltd, 2nd edn, 2008.
8. Photochemistry and Pericyclic Reactions, J. Singh and J. Singh, Third Edition, New Age International (P) Ltd, 2012.

MCYC 203 Physical Chemistry-II (3-0-0) (3 credits)

Module-I (12 hours)

Chemical Kinetics: Complex reactions –opposing , parallel and consecutive reactions. Mechanism of reactions. Chain reactions –linear reactions, branching chains– explosion limits; Rice Herzfeld scheme.

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, Kramers theory. Diffusion limited reactions.

Study of fast reactions using stopped flow and relaxation techniques.

Module II (12 hours)

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.

Surface phenomena: Amphiphilic molecules and 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.

Module III (10 hours)

Physical Photochemistry: Franck-Condon Principle, Laws of Photochemical Equivalence.
Unimolecular Photophysical Processes: vibronic transitions, Kasha's rule, fluorescence and phosphorescenece, internal conversion, intersystem crossing. Mirror symmetry relationaship, fluorescence life-time, quantum yields of various processes.
Bimolecular Photophysical Processes: Photoinduced electron-transfer and charge transfer processes, excimer and exiplex, fluroscence quenching. Radiative, Forster type and Dexter type enegy transfer.

Text Books (**Physical Chemistry_II**)

1. Chemical Kinetics-K. J. Laidler, pearson Education,2004
2. D.A. McQuarrie and J. D. Simon : Physical Chemistry - A Molecular Approach
3. Fundamentals of Photochemistry- K. K. Rohatgi-Mukharjii, Wiley Eastern

Reference Books

1. Elements of Physical Chemistry, P. Atkins and J. de Paula, 6th edn, Oxpord Press, 2015.
2. Photochemistry – J. G. Calverts and J. N. Pitts, John-Wiley & Sons
3. J. R. Lakowicz, Principles of Fluorescence Spectroscopy

MCYC204 Spectroscopic Identification of Molecules (3-1-0) (4 credits)

Module I (12 hours)

Introduction to spectroscopic techniques of structure elucidation. Electromagnetic radiation, energy and electromagnetic spectrum, units, absorption of energy by organic compounds, types of spectroscopic methods to organic structure elucidation.

IR – Spectroscopy – Basic principles, characteristic frequencies of common functional groups.

UV – Visible Spectroscopy: Basic principles, application of UV – Visible spectroscopy to organic structure elucidation, Woodward – Fisher rules.

Module II (12 hours)

Nuclear Magnetic Resonance Spectroscopy: Application of ^{1}H and ^{13}C NMR spectroscopy including COSY, NOESY, NOE techniques in the structural determination of complex organic systems and NMR of common heteroatoms present in organic compounds (N, F, O, P, S and D). Applications in conformational analysis. Multinuclear NMR of various inorganic and organometallic compounds.

Electron Spin Resonance Spectroscopy: Analysis of ESR spectra of systems in liquid phase, radicals containing single set, multiple sets of protons, triplet ground states. Transition metal ions.

Double resonance techniques: ENDOR in liquid 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.

Module III (8 hours)

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.

Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules. Isotope effects and basics of HRMS, and its necessity in organic synthetic chemistry field.

Module IV (8 hours)

Problem solving exercises involving UV, IR, NMR & MS data: Problems involving interpretation of spectral details of organic compounds .

Text Books:

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).

R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds., John Wiley and Sons.Inc., Sixth edition (1997).

Reference Books

W. Kemp, Organic Spectroscopy, Third Edition , MacMillon (1994).

Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks/Cole Pubs. Co.

D. H Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, (1998).

William Kemp, Introduction to multinuclear NMR.

MCYF205 Chemical Biology (3-0-0) (3 credits)

Module -1 (20 hrs)

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; replication, transcription and translation.

Structure and function of Hormones, Minerals and Vitamins; Bio-complexes: Nucleoproteins, Glyco-proteins, Lipoproteins and Vitamin complexes.

Module-II (8Hr.)

Principle of Bioenergetics: Bioenergetics and Thermodynamics; Phosphoryl group transfer and energy currency-ATP; Biological Oxidation and reduction reactions

Metabolic processes: Introduction to metabolism of carbohydrates: Glycolysis, TCA Cycle, Gluconeogenesis.

Module-III (10 hrs)

Transport Mechanism

Na^+/K^+ transport (Ion pump); O_2 transport by hemoglobin, CO_2 transport by carbonic anhydrase.

Enzymes: Properties of enzyme, classification of enzymes, mechanism of enzyme action, kinetics of of ienzyme 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, C.B.Powar & G.R.Chatwal, Himalaya Publishing House.
5. Biochemistry, Rastogi, Tata McGraw Hill.

MCYC250 Analytical Chemistry Laboratory (0-0-6) (3 credits)

I. Spectroscopic determination of:
   - Iron/ copper/ nickel in minute quantities by UV-Vis spectrophotometry
   - Principles of colorimetric analysis: determination of iron content of an unknown sample.

II. Spectroscopic determination of:
   - Phosphate in water sample and cola drinks
   - Chromium(VI) in water sample

III. Determination of composition of a complex using Job's method

IV. Thermal decomposition of $CuSO4.5H_2O$

V. Redox behavior of potassium ferricyanide by cyclic voltammetry

Selected Text/Reference Books:

1. G., Svehla, Vogel's Qualitative Inorganic Analysis, 6th Edn., Orient Longman New Delhi, l987.
2. V.V. Ramanujam, Inorganic Semi-micro Qualitative Analysis, 3rd Edn., National Publishing Company, Madras, l990.
3. J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny,Vogel's text book of Quantitative Chemical Analysis, 5th Edition, Longman Scientific and Technical (1999).
4. Hand-outs prepared for the laboratory experiments: collections from various literature sources
5. Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press, (India) Pvt. Ltd., 2002.
6. Roesky, H. W.; Möckel, K., Chemical Curiosities: spectacular experiments and inspired quotes, VCH, 1996.

2nd semester

MCYC251 Physical Chemistry-I Laboratory (0-0-3) (3 credits)

1. pH metry / conductometry / potentiometry and precipitation titrations.
2. Spectrophotometric determination of the acid dissociation constant.
3. Inversion of sucrose using polarimeter.
4. Determination of critical miceller concentration of surfactants.
5. Polarizability from refractive index measurements.
6. Composition of a complex by Job's method.

Text Books

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

References

1. B. B. Dey, and M. V. Sitharaman, 'Laboratory Manual of Organic Chemistry' Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi. 4th Revised Edn. l992.

MCYF252 Computational Chemistry Laboratory (0-0-6) **(3 credits)**

Programming Lab-1

Module – I

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, Input-output statements, if and switch statements, loops:-while, do-while and for statements, break, continue, etc.

a) Write a C program to find the sum of individual digits of a positive integer.
b) Write a C program to find Fibonacci sequence.
c) Write a C program to generate all the prime numbers between 1 and n.
d) Write a C program to find the roots of a quadratic equation.
e) Write a C program to find both the largest and smallest number in a list of integers.

Module – II

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, Pointers- concepts, initialization of pointer variables, pointers and function arguments, address arithmetic, Character pointers and functions, pointers to pointers, Dynamic memory management.

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.
b) Write a C program that uses functions to perform the following:
    i) Addition of Two Matrices
    ii) Multiplication of Two Matrices
c) 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.
d) Write a C program to determine if the given string is a palindrome or not
e) Write a C program to construct a pyramid of numbers.

Module – III

Derived types- structures- declaration, definition and initialization of structures, accessing structures, nested structures, arrays of structures, structures and functions, pointers to structures, union.

a) Write a program to display Name, Roll Number, Marks of different subjects etc. of n number of students.
b) Write a C program to count the lines, words and characters in a given text.
c) Write a C program that uses structure 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.)

Module-IV

Use of Gaussian software to find the bond length and bond angle of some simple molecules like H_2O, NH_3, CH_4 and CCl_4 using suitable theoretical approaches.

3rd Semester

MCYC 301 Analytical Techniques –I (3-0-0) (3 credits)

Module I (8 hours)

Tools and Data Handling: Balances, burettes, volumetric flasks, pipettes, calibration of tools, sampling. Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, confidence limit, test of significance, rejection of a result.

Module II (8 hours)

Separation Techniques: Solvent Extraction: distribution Coefficient, distribution ratio, solvent extraction of metals, multiple batch extraction, counter current distribution. - Chromatographic Techniques: classification, theory of chromatographic separation, distribution coefficient, retention, sorption, efficiency and resolution. - Column, ion exchange, paper, TLC & HPTLC: techniques and application. - Gas Chromatography: retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

Module III (10 hours)

Spectroscopic Techniques: Electromagnetic radiation, absorption, and emission of radiation – instrumentation: sources, monochromators, detectors. - Flame spectrometry: flame emission, AAS, ICP, instrumentation and application. - Absorption spectrometry: UV-VIS, IR, instrumentation, techniques and applications.

Textbook:

1. D. C. Harris, Quantitative Chemical Analysis, 4th Ed., W. H. Freeman, 1995

Further reading:

2. G. D.Christian & J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn & Balon, 1986.
3. D. A. Skoog, F. J. Holler, S. R. Crouch, Instrumental Analysis, Cengage Learning, 11th edn., 2012.

MCYC 302 Organic Chemistry-III (3-0-0) (3 Credits)

Module I (12 hours)

Green Chemistry: Principles, green solvents, concepts of atom economy, Domino and multi component reactions, green synthesis of pharmaceuticals and industrial chemicals.

Coupling Reactions: Carbon-carbon bond formation through coupling reactions (Heck, Suzuki, Stille and Sonogoshira), Carbon-hetero atom bond forming reactions using transition metals (Cu,Pd, Rh, Ru, Ni, Fe etc.)

Rearrengements:

General mechanistic considerations- nature of migration, migratory aptitude, memory effects,
A detailed study of the following rearrengements: Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Bayer-Villiger, Shapiro reaction. Free-radical rearrangement reactions.

Oxidation:

Introduction to various oxidative processes:
Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated), alcohols, diols, aldehydes, ketones, ketals and carboxylic acids, amines, hydrazines, and sulfides, oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate.

Reduction:

Introduction to various reductive processes:
Alkenes, alkynes and aromatic rings, carbonyl compounds (aldehydes, ketones, acids and their derivatives), epoxides, nitro, nitroso, azo and oxime groups, hydrogenolysis.

Synthetic Strategies:

Umpolung reactivity – formyl and acyl anion equivalents. Selectivity in organic synthesis – chemo-, regio- and stereoselectivity. Concepts of asymmetric synthesis – resolution (including enzymatic), desymmetrization and use of chiral auxilliaries. Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silyl enol ethers. Michael addition reaction. Stereoselective addition to C=O groups (Cram and Felkin-Anh models).

Heterocyclic Compounds:

Introduction to heterocycles, nomenclature, structure, preparation, properties and reactions of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline.

Text and Reference Books:

1. Advanced Organic Chemistry Part A & B:, Carey, F. A., Sundberg, R. J, Fifth Edition, Springer International Edition.
2. Principles of Organic Synthesis, R. O. C. Norman and J.M.Coxon, Third Edition, Blackie Academic and Professional
3. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, Jerry March, Sixth Edition, John Wiley & Sons, Inc.
4. Organic Synthesis: Clayden J., Greeves N, Warren S, and Wouthers, Second Edition Oxford University
5. Heterocyclic Chemistry, Thomas. L. Gilchrist, Third Edition, 1997
6. Heterocyclic Chemistry, Joules J.A., Mills K., Smith G.F., Third Edition.
7. Advances in Heterocyclic Chemistry, Book Series Elsevier Edited by Alan Katritzky
8. Green Chemistry and Catalysis, Sheldon R.A., Arends I., Hanefeld Ulf, Wiley-VCH.
9. Green Chemistry: Theory and Practice, Anastas P.T, Warner J.C
10. New Trends in Green Chemistry, Ahluwalia V. K., Kidwai M.

MCYF 303 Environmental Chemistry (3-1-0) (4 credits)

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, Advanced oxidation process.

Module – II (14 Hours)

(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 (14 Hours)

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.

MCYF 304 Materials Chemistry (3-0-0) (3 credits)

Module I (10 Hours)

Materials and their classification: Matter, materials science, broad classification of materials, -metal and alloys, polymers and elastomers, ceramics and refractories, semiconducting 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.

Module II (10 Hours)

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 III (8 Hours)

Dielectric and Magnetic Materials: 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 IV (8 Hours)

Dielectric and Magnetic Materials:

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.

Recommended Books:

1. Magnetic and Dielectric Properties of Materials: Basics, Theories and Experiments – by Mohammad Mahbubur Rahman, 2012
2. Chemical Processing of Advanced Materials: L. L. Hench and J. K. West (eds), John Wiley New York 1992.
3. P. Hagnmuller (ed): Preparative Methods in Solid State Chemistry, Academic Press, New York, 1972.
4. Sol-Gel Science, C. J. Brinker & G. W. Scherer, Academic Press, 1980.
5. Non-Oxide Technical & Engg. Ceramics, Ed. Stuart Hampshire, Elsevier Applied Science Pub. Ltd. 1986.
6. Semiconductor Material and Device Characterization , by Dieter K. Schroder, Springer, 3rd edition 2006.
7. Introduction to Semiconductor Materials and Devices by M.S.Tyagi , John Wiley & Sons, 2008
8. The Materials Science of Semiconductors by Angus Rockett Springer, 2008
9. Ultrastructure Processing of Ceramics, glasses and Composited, Ed. L. L. Hench, D.R. Ulrich, John Wiley, New York 1984.

MCYF 305 Solid State Chemistry (3-0-0) (3 credits)

Module I

Chemical crystallography (14 hours)

Introduction, Space lattice, Crystal point groups, space group (working knowledge), Stereographic projections, Packing in solids, Crystal structures of representative systems, Silicates and Zeolites, Cements, Glasses, Quasicrystals, Nanostructures.

Bonding in solids and Crystal energetics

Crystal classifications, Madelung constant and Lattice energy.

Module II (12 hours)

Electronic properties and Band theory of solids

Free electron model, Metals, semiconductors and insulators, doped semiconductors
Solid state ionics.

Defects, Nonstoichiometry and Diffusion

Point defects, Dislocations, Extended defects, Clusters and aggregates, Color centres, Non-stoichiometry of compounds, Diffusion mechanisms, Fick's law, Kirkenall effect.

Phase transitions

Critical phenomena, variety of phase transitions (Ordered- disorder, Martensite-austenite, Spinoidal decompositions etc), Liquid crystals, Structure-property relations (magnetic, electrical, superconductivity, optical and thermal).

Module III

Preparative and characterization techniques (14 hours)

Powder synthesis by conventional and modern chemical methods, Reactivity of solids, Decomposition mechanisms, Powder processing (sintering and diffusion processes), Tailoring of solids, Special methods for single crystal growth and thin films depositions.

Characterization techniques (working knowledge) for solids

X-ray diffraction, Electron microscopy (SEM, TEM, AFM), Spectroscopic techniques (Mossbauer, IR, UV-VIS) and Physical property measurement techniques (Magnetic moments-VSM /SQUID, Electrical resistivity – Two / Four probe methods and thermal conductivity, Optical band gap, XPS, XAS).

Recommended books:

1. A. R. West, Solid State chemistry and its applications, 2nd edition, John Wiley & Sons,.
2. L. Smart and E. Moore, Solid State chemistry: An Introduction, 4th edition, Chapman and Hall.
3. A. K. Cheetham and P. Day, Solid state chemistry compounds, Clarendon Press, Oxford 1992.
4. C. N. R. Rao and J. Gopalkrishanan, New directions in solid state chemistry, Cambridge Univ. 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

MCYC 350 Physical Chemistry-II Lab (0-0-6) (3 credits)

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 (0-0-3) (2 credits)

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 Chemical Biology laboratory (0-0-3) (2 credits)

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.

MCYC301 Organometallic Chemistry

MODULE-I **(14 Hours)**

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 complexation with 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 **(14 Hours)**

Addition and abstraction: Nucleophilic addition to CO, 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,
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.

MCYC302 Chemistry of Drug Design

Module I

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

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 **(14 Hours)**

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, Diamino Pyrimidines, 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 , sulfonyl ureas, hazards and side effects.

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

Books:

5. The Organic Chemistry of Drug Design and Drug Action – by Richard B. Silverman &, Mark W. Holladay = 3rd edition- 2014- Academic Press
6. Medicinal Chemistry: A Biochemical Approach, Thomas Nogrady
7. Drug Discovery Strategies and Methods by Alexandros Makriyannis, Diane Biegel, 2003, CRC press
8. Textbook of Drug Design and Discovery, -edited by Tommy Liljefors, Povl Krogsgaard-Larsen, Ulf Madsen -Third Edition-– CRC press
9. Drug Design Strategies = David J Livingstone , Andrew M Davis –RSC publishing- 2011
10. Drug Design by Klebe Gerhard by Springer

7 . Principles of Medicinal Chemistry, William O. Foye

8. The Pharmacological Basis of Therapeutics: Goodman and Gilman

9. Introduction to Drug Metabolism, G. Gordon Gibson and Paul Sket

MCYF301 Environmental Chemistry
MCYF302 Chemical Synthetic Strategy of Advanced Materials & Nano materials
Module-III: Semi-Conductor and Electronic Materials. (14 Hours)

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.

Recommended Books:

1. Magnetic and Dielectric Properties of Materials: Basics, Theories and Experiments – by Mohammad Mahbubur Rahman, 2012

5. Chemical Processing of Advanced Materials: L. L. Hench and J. K. West (eds), John Wiley New York 1992.
6. P. Hagnmuller (ed): Preparative Methods in Solid State Chemistry, Academic Press, New York, 1972.
7. Sol-Gel Science, C. J. Brinker & G. W. Scherer, Academic Press, 1980.
   Non-Oxide Technical & Engg. Ceramics, Ed. Stuart Hampshire, Elsevier Applied Science Pub. Ltd. 1986.

11. Ultrastructure Processing of Ceramics, glasses and Composited, Ed. L. L. Hench, D.R. Ulrich, John Wiley, New York 1984.

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 to chemistry : statistical thermodynamics, chemical kinetics, Curve fitting, Gaussian and Lorentzian deconvolution

Use of software packages such as visualization, semi-empirical methods.

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. Gausssian Sofetware

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. Michael Boillot, Understanding Fortran77, wess-publishing company, New York(1987).
5 Fortran95/2003 for scientists and engineers, S.J.Chapman, McGrawHill 2008).
6. S.C.Chapra and R.P.Canale, Numerical Methods for Engineers, Tata McGraw Hill, New Delhi (2003).

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 Analytical Chemistry-II (3-0-0)

Module I (12 hours)

Thermal Techniques:
Thermogravimetry (TG), Differential gravimetric analysis (DTG) and Differential thermal analysis (DTA- instrumentation and techniques,
Radiochemical methods: decay reactions, growth of radioactivity, radiation detectors, tracer techniques.

Module II (14 hours)

CD and Fluorescence specroscopy

Module III **(14 hours)**

Electroanalytical Techniques: Electrogravimetry, coulometry, voltam- metry, polarography, conductometry, instrumentation, techniques and application.

Module IV **(10 hours)**

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, 3rd edn., 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 coordination polymerisation (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)

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 colour centres 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 and Characterization of Materials

Module-I Introduction **10 hours**

Historical Perspective, Material classification: Electronic materials, optical materials, ceramic materials, electro chemical materials.

Module-II Material synthesis **16 hours**

Synthesis of bulk Polycrystalline Materials: Direct combination, chemical precursor methods, reactive thermal evaporation, sono-chemical methods of nano-material synthesis, co-precipitation method, Sol-gel technique, nano-phase materials, composites, high pressure and high temperature techniques. Bulk Single Crystal Materials: Principles and methods: melt and flux techniques, chemical vapors transport techniques: hydrothermal synthesis: growth by fused salt electrolysis: Zone refining.

Module-III Characterization Techniques and Applications **14 hours**

Destructive Techniques: Principles of chemical analysis, DTA, TGA, DSC. Non-destructive Techniques: use of x-ray electron and neutron diffraction techniques. Applications of material in heterogeneous catalysis, textiles and fabric, health care.

Essential Readings

1. Materials Synthesis and Characterization, Dale L. Perry, Springer; reprint of the original 1st ed. 1997 edition, 2013.
2. Materials Science and Engineering: An Introduction, William D. Callister, Jr., John Wiley & Sons, Inc., 7^{th} edition, 2007
3. Synthesis and Characterization of Advanced Materials, National Academy Press, Washington D. C., 1984 **http://www.nap.edu/catalog/10846.html**

MCYF 406 Supramolecular Chemistry

Module I (12 hours)

Introduction-the meaning of supramolecular chemistry, phenomenon of molecular recognition and their quantification

Building blocks of supramolecular chemistry- acyclic receptors for neutral and charged guests, macrocycles and crown ethers, macrobicycles and cryptands, macropolycycles, cucurbiturils and cyclodextrins

Module II (15 hours)

Sensors and information processing, electro-optic phenomena, molecular machines

Amphiphilic molecules and their aggregation, Langmuir-Blodgettry, molecular recognition at the air-water interface.

Module III (13 hours)

Discrete and polymeric metal-organic hybrid materials- guest inclusion, catalysis and other applications.

Books

1. Supramolecular Chemistry: Concepts and Perspectives, J.-M. Lehn, VCH, Weinheim, 1995
2. Principles and Methods in Supramolecular Chemistry, H. J. Schneider and A. Yatsimirsky, Wiley, New York, 2000
3. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley & Sons, Chichester, 2009
4. Ariga, Katsuhiko & Kunitake, Toyoki, Supramolecular Chemistry - Fundamentals and Applications , 2006, Iwanami Shoten Publishers, Tokyo

MCYF 407 Chemistry of Natural Products

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)

Biosynthetic aspects and Synthesis of selected natural products of biological and structural 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 in Total Synthesis" Vols I-III, Wiley-VCH, 1996; 2003; 2011
2. T. Hudlicky and J. W. Reed, "The way of synthesis" , Wiley-VCH, 2007
3. E. J. Corey and X-M. Cheng, "The logic of chemical synthesis, John-Wiley & Sons, New York, 1989.
4. D.H. R. Barton, K. Nakanishi, O. Meth-Cohn, "Comprehensive natural products chemistry" Vols 1-9, Elsevier, 1999.
5. N. R. Krishnamurty, Chemistry of Natural Products, University Press, 2nd edition 2010.

MCYF 408 Frontiers in Organic Chemistry

Module I (10 hours)

Green Chemistry, Glycobiology, Synthetic aspects using Domino reactions, Principles of atom economy with examples.

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, "Essentiall of carbohydrate chemistry and biochemistry, Wiley-VCH, 2006

2. Farges, Organic Conductors: Fundamentals and Applications (Applied Physics), CRC press, 1994

1. Sambhu N Datta **&** Francesc Illas **,** Theoretical and Computational Aspects of Magnetic Organic Molecules, 2014, world scientific.
2. Jan Kalinowski, Organic Light-Emitting Diodes: Principles, Characteristics & Processes (Optical Science and Engineering) Hardcover – CRC press, 2004

3. J. Tsuji, "Transition metal reagents and catalyst innovations in organic synthesis" John-Wiley-& Sons, Ltd, New York, 2000
4. W. Bannwarth, B. Hinzen, Combinatorial Chemistry - From Theory to Application Wiley-VCH, 2nd edition, 2006.
5. Michael Pirrung, Molecular Diversity and Combinatorial Chemistry, Elsevier, 2004.
6. 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)

Reductive cleavage of dioxygen bond, biological dioxygen carriers, dioxygen reactions, cytochrome c oxidase, cytochrome p-450, catalase, peroxidase, Cu-Zn superoxide dismutase. Novel organic transformations 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. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, University Science Books, Mill Valley, 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: Review of kinetic theory of gases, collisions - atomic and molecular.

Rate theories :Transition state theory and RRKM theory, scattering phenomena- classical and quantum.

Oscillatory Reactions: Theory with examples.

Module II (12 hours)

Reactive Collisions: Potential energy surfaces, atom-diatom reactions, polyatomic reactions, state-selective, molecular beams, reaction rates and cross sections.

Module III (16 hours)

Dynamics in gas phase :Photodissociation, energy transfer, stereodynamics, chemistry in real time with lasers, control.

Dynamics in condensed phase : Solvation, diffusion, barrier crossing, Kramer-Grote-Hynes theory, Langevin equation, correlation functions.

Recommended Books

1. Levine, Molecular Reaction Dynamics, 2005.
2. Henriksen & Hansen, Theories of Molecular Reaction Dynamics, 2008.
3. Schinke, Photodissociation Dynamics, 1993.
4. Manz & Wöste, Femtosecond Chemistry, 1995.
5. Nitzan, Chemical Dynamics in Condensed Phases, 2006.

MCYF 411 Enzyme: Reactions Mechanism and Kinetics

Module I **(12 hours)**

Enzyme kinetics of single and multiple substrate systems including Enzyme assays and inhibition .

Module II **(12 hours)**

Cooperativity and multienzyme systems.

Enzyme structure and identification of active site residues labelin, chemical modification and mutagenesis.

Module III **(14 hours)**

Enzyme Mechanisms – Methods of study and mechanisms of some enzymes like

Serine proteases, polymerases, ribonucleases, lysozyme and ribonucleotide reductases (radical enzyme).

Mechanism based enzyme inhibition and drugs –5-fluorouracil for thymidylate synthase.

Books:

1.Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding by Allan Ferhst

2. N. C. Price and E. Stevens, Fundamentals of Enzymology: The Cell and Molecular Biology of Catalytic Proteins

3. I. H. Sigel, Enzyme Kinetics: Behavior and Analysis of Rapid Equilibrium and Steady-State Enzyme Systems, John Wiley & Sons, 1993.

5. Herbert M. Sauro, Enzyme Kinetics for Systems Biology, Wiley 2012
6. 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

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