OFFICE OF THE REGISTRAR:: DIBRUGARH UNIVERSITY:DIBRUGARH

Memo No. DU/DR-A/7-1/14/504 Date: 01.08.2014.

NOTIFICATION

As recommended by the Board of Studies in Chemistry, Dibrugarh University held on 13.05.2014, the hon'ble Vice-Chancellor, Dibrugarh University is pleased to approve the draft of the Course Structure and Syllabus for the Four Semester M.Sc. Programme in Chemistry under Choice Based Credit System under report to the Post Graduate Board, Dibrugarh University.

The syllabus shall come into effect from the 2014-2015 Academic Session.

Sd/-B.C. Borah
Deputy Registrar (Academic)
Dibrugarh University

Copy to:

1. The Vice-Chancellor, Dibrugarh University.
2. The Registrar, Dibrugarh University.
3. The Controller of Examinations, Dibrugarh University, for favour of information and needful. A copy of the approved syllabus is enclosed.
4. The Head, Department of Chemistry, D.U. Dibrugarh, for favour of information and needful. A copy of the approved syllabus is enclosed.
5. File.

Sd/-B.C. Borah
Deputy Registrar (Academic)
Dibrugarh University.

Post Graduate Syllabus in Chemistry

for

Four Semester M.Sc. Course (2 Years)

under

Choice Based Credit System (CBCS)

(Revised on 12.05.2014)

Department of Chemistry

Dibrugarh University

Dibrugarh – 786 004

Assam, India

Department of Chemistry: Dibrugarh University

M.Sc. Syllabus in Chemistry under Choice Based Credit System (CBCS)

(Revised on 12.05.2014)

1. Name of the Course: M.Sc. (Chemistry) – Four Semester System

2. Structure of the syllabus in terms of Number of papers, Credits and Marks

Structure of the syllabus									
	Number of Paper			**Credit**			**Marks**		
	Theory	Practical	**Total**	Theory	Practical	**Total**	Theory	Practical*	**Total**
Semester I									
	5	1	**06**	18	06	**24**	450	150	**600**
Semester II									
	5	1	**06**	18	06	**24**	450	150	**600**
Semester III									
	5	1	**06**	17	06	**23**	425	150	**575**
Semester IV									
	5	1	**06**	13	08	**21**	325	200	**525**
Total number of Paper			**24**	**Total Credit**		**92**	**Total Marks**		**2300**

*In Semester IV, it is Advance practical/Project

3. (i) Each theory paper will carry 40% Internal Assessment (Seminar + Home Assignment + In-semester test) of the total marks in the said paper

(ii) Each practical/ Lab work/ Project paper will also carry 40% Internal Assessment which includes attendance, performance in the laboratory.

(iii) 25 marks will be equivalent to 1 credit for all courses

4. (a) Total Credits :- 92 (Theory + Practical)

(b) Total Marks: - 2300 (Theory+ Practical)

[1 Credit equivalent to 25 marks]

5. Structure of the course:

	Semester I		
Course	Course title	Credit	Marks (End Semester+ Internal Assessment)
10100	Inorganic & General Chemistry	4	100 (60+40)
10200	Principles of Organic Chemistry	4	100 (60+40)
10300	Physical Chemistry I	4	100 (60+40)
10400	Quantum Chemistry	3	75 (45+30)
10500	Spectroscopy I	3	75 (45+30)
10600	Practical	6	150 (90+60) [Experiment=70, Viva=20]
	Total	**24**	**600**

	Semester II		
Course	Course title	Credit	Marks (End Semester+ Internal Assesment)
20100	Chemistry of Transition metals and Materials Chemistry	4	100 (60+40)
20200	Bioorganic and Heterocyclic Chemistry	4	100 (60+40)
20300	Physical Chemistry II	4	100 (60+40)
20400	Symmetry & Group Theory	3	75 (45+30)
20500	Spectroscopy II	3	75 (45+30)
20600	Practical	6	150 (90+60) [Experiment=70, Viva=20]
	Total	**24**	**600**

	Semester III		
Course	Course title	Credit	Marks (End Semester+ Internal Assessment)
30100	Advanced Inorganic Chemistry	4 (3L+1T)	100 (60+40)
30200	Advanced Organic Chemistry	4 (3L+1T)	100 (60+40)
30300	Physical Chemistry III	4 (3L+1T)	100 (60+40)
30400	Advanced Topics in Chemistry (Computational Chemistry, Biochemistry and Supramolecular Chemistry)	3	75 (45+30)
30500	Petrochemical Process Technology	2	50 (30+20)
30600	Practical	6	150 (90+60) [Experiment=70, Viva=20]
	Total	**23**	**575**

	Semester IV		
Course	Course title	Credit	Marks (End Semester + Internal Assessment)
40100	Physical Methods in Chemical Analysis	3	75 (45+30)
40200	Green Chemistry	1	25 (15+10)
40300	Research Methodology	1	25 (15+10)
*	Special Paper I*	4 (3L+1T)	100 (60+40)
*	Special Paper II*	4 (3L+1T)	100 (60+40)
40800	Advanced Practical/ Project	8	200 (120+80) [Experiment=70, Literature Review=20, Viva=30]
	Total	**21**	**525**

L=Lecture; T= Tutorial/Remedial/Counseling

***These have to be opted from a set of Elective I, II, III, IV (any two to be opted) of each specialization (details are following).**

Details of the elective courses.

Course		Course title
Elective I	40410	Inorganic reaction mechanism and kinetics
	40420	Organic Synthesis
	40430	Advanced Polymer Chemistry
Elective II	40510	Transition metal organometallics and Metal clusters
	40520	Natural Products Chemistry
	40530	Advanced Electrochemistry
Elective III	40610	Bio-inorganic Chemistry
	40620	Bioorganic Chemistry and Biochemistry
	40630	Solid State Chemistry
Elective IV	40710	Introduction to Chemistry of Nanomaterials
	40720	Medicinal Chemistry
	40730	Advanced Quantum Chemistry

Any two papers to be opted from Elective I, II, III, IV from the same specialization.

(e.g. a students may opt for **two papers** from **any of the following sets** (Specialization)

Set I (Specialization : Inorganic) **: 40410, 40510, 40610, 40710**

Set II (Specialization : Organic) **: 40420, 40520, 40620, 40720**

Set III (Specialization : Physical) : **40430, 40530, 40630, 40730**

SEMESTER I

Course: 10100
Inorganic & General Chemistry
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit-I Chemical Bonding & Electronegativity

LCAO-MO methods in homo and heteronuclear diatomic molecules (O_2, N_2, CO, NO). MO description of tri and tetraatomic molecules (CO_2, NO_2, NO_2^+, CO_3^{-2}, O_3 and NO_3^-).

Metallic bonding: Band theory of Solids – conductor, semiconductor and insulators. Superconducting oxides. Spinel and Perovskite structures.

VSEPR Theory: Structure of molecules containing lone pair(s) of electrons, structure and hybridization, Bent's rule, Bent bond, Non-bonded repulsion and structure.

Mulliken-Jaffe electronegativity scale, spectroscopic electronegaitvity, Absolute and group electronegativity. Chemical hardness, Application of electronegativity. Marks 15

Unit-II : Acid Base and Redox Chemistry

Acid-Base concepts, Measure of Acid-Base Strengths, Acid-Base in water. Non-aqueous solvent, aprotic solvent and superacids. Hard and Soft Acids and Bases, application of SHAB principle.

Half cell reaction, reduction potential, application of reduction potential data, electrochemical series; brief idea of corrosion and its prevention; Nernst equation. Latimer and Frost diagram, disproportionation reaction; cyclic voltametry. Marks15

Unit-III: Bioinorganic and environmental Chemistry

Fundamentals of inorganic biochemistry, essential and non-essential elements in bio-systems. Natural and synthetic oxygen carriers, model compounds for oxygen carriers, carboxy-peptidases, chlorophyll and photosynthesis, Na-K or ATPase or sodium pump, crown ethers, futuristic aspects of organo-transition metal complexes in bioinorganic chemistry.

Poisioning effect due to non-metals, toxic effects of oxides of carbon, nitrogen and sulphur. Acid rain; poisioning effect due to Nitrite; CFC's, O_3- layer depletion; Heavy Metal pollution (Hg and Pb). Smog pollution, Renewable resources of energy. Plastic Pollution and its prevention. Marks: 18

Unit-IV:

Bonding in electron deficient compounds. Structure and bonding in boranes, carboranes, metallocarboranes, S-N and Se-N and P-N compounds.

Aluminosilicates, zeolites and molecular sieves. Fullerene (C_{60}) Marks12

Recommended Texts:

1. Bioinorganic Chemistry by K. Hussain Reddy, New Age International Publisher.
2. The Inorganic Chemistry of Biological Processes, Hughes, M.N., 2nd edition, Wiley (1981)
3. Bio-coordination Chemistry, D.E. Fenton, Oxford University Monograph Series 1995.
4. Inorganic Chemistry, Gary L.Miessler & Donald A. Tarr 3rd Ed, Pearson
5. Inorganic Chemistry, C.E. Housecraft & A.G. Sharpe, 2nd Ed, Pearson

Course: 10200
Principles of Organic Chemistry
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit I

Structure, bonding and reactivity of organic compounds : Aromaticity, antiaromacity and homoaromaticity, metallocenes, tropolones and azulenes. Bonds weaker than covalent bond – charge transfer complexes, inclusion complexes and crown ethers. Cryptand, rotaxanes, Fullerenes, Graphenes. Phase transfer catalyst.

Hammet equation, Taft equation. Influence of reaction medium on rates

HSAB concepts and their applications. *Marks 15*

Unit II

Organic reaction mechanism – Transition state vs. Reaction intermediate, Energy profile of multistep reaction, Significance of rate limiting step in multistep reactions, Catalysed and uncatalysed reactions, Kinetic vs. Thermodynamic control, Kinetic and non-kinetic methods of studying organic reaction mechanism; Isotope labeling studies and kinetic isotope effects, Cross-over experiment. Reactivity - selectivity principle : Chemoselectivity, regioselectivity, stereoselectivity and stereospecificity in substitution, elimination and addition reactions. Neighbouring group effects. *Marks 15*

Unit III

Stereochemistry– Molecular symmetry, asymmetry and dissymmetry; Classification of organic molecules into different point groups, Concept of prostereoisomerism and prochirality – Homotopic and heterotopic ligands and faces; Optical purity and enantiomeric excess; Chirality in molecules devoid of chiral centers - allenes, spirans and biphenyls.

Classification of stereoselective synthesis: diastereoselective and enantioselective reactions; Stereo-differentiating approach, Nucleophilic addition to aldehydes and acyclic ketones: Cram and Felkin – Ahn model. Enantioselective synthesis – Use of chiral reagent, chiral catalyst and chiral auxillary. *Marks-15*

Unit IV

Disconnection approach in organic synthesis: Retrosynthesis of Alcohols (Grignard approaches and hydride transfer approaches) and Carbonyl compounds. Acceptor and donor synthons, Use of umpolung, One group and two group C-X disconnections. One group and two group C-C disconnections. Retrosynthsis of 1,2-, 1,3-, 1,4-, 1,5- and 1,6- difunctional (O,O and N,O in a difunctional relation) compounds.

Use of protecting groups in organic synthesis : protection and deprotection of hydroxyl, dihydroxy, carbonyl, carboxyl and amino groups. *Marks-15*

Recommended books

1. Organic Chemistry, Vols I and II – I. L. Finar, ELBS.
2. Organic Chemistry – R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Prentice Hall India Limited
3. Organic Chemistry – Paula Yurkanis Bruice, Pearson
4. Advanced Organic Chemistry: Reaction Mechanism and Structure – Jerry March, Wiley Eastern.
5. A Guidebook to Mechanism in Organic Chemistry– Peter Sykes, Longman, New York.
6. Stereochemistry of Organic Compounds – D. Nasipuri, Wiley Eastern
7. Stereochemistry of Carbon Compounds – Earnest E. Eliel, Tata McGraw Hill
8. Stereochemistry of Carbon Compounds – Subrata Sengupta, New Central Book agency, Kolkata
9. Stereochemistry and Mechanism through Solved Problems- P.S. Kalsi, New Age International Publishers
10. Disconnection Approach in Organic Synthesis – S. Warren, Wiley
11. Organic Reaction Mechanism, Christine Willis and martin Willis, Oxford chemistry Primers (No. 74)
11. Disconnection Approach in Organic Synthesis – S. Warren, Wiley
12. Designing Organic Synthesis – S. Warren, Wiley, Chichester
13. The Logic of Organic Synthesis – E.J. Corey and Xue Min Chen, Wiley, New York

Course: 10300
Physical Chemistry I
(Equilibrium, Non-equilibrium and Statistical Thermodynamics)
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Group A

Equilibrium and Non-equilibrium Thermodynamics (Marks 30)

Unit I: Equilibrium thermodynamics:

Concept of fugacity and it determination. Ideal solution and non ideal solutions, Activity and activity coefficient, Determination of activity coefficient, excess function for non-ideal solutions. Partial molar quantities: chemical potential, Determination of partial molar

volume, Thermodynamics of mixing. Third law of thermodynamics, its experimental verification, determination of absolute entropy. *Marks 12*

Unit II: Non-equilibrium thermodynamics:

Difference between equilibrium and non-equilibrium thermodynamics, Criteria of non-equilibrium thermodynamics; uncompensated heat and its relation to other thermodynamic functions, Fluxes and forces- relation between these two quantities, Entropy production in heat transfer, mass transfer in flow of current, in mixing of gases, and in chemical reaction; phenomenological relation: Onsagar relation, microscopic reversibility and Onsager reciprocity. Coupled reaction. Thermoelectric effects: Seebeck, Peltier and Thompson effect.

Marks 18

Group B

Statistical Thermodynamics (Marks 30)

Unit I

Probability and most probable distribution, distribution of non distinguishable particles, Striling theorem, Maxwell-Boltzmann distribution law, Bose-Einstein and Fermi-Dirac distribution law. *Marks 5*

Unit II

Boltzmann relation between entropy and probability. Partition functions and thermodynamic functions. Thermodynamic functions of a monatomic gas, Sackur – Tetrode equation. Evaluation of translational partition function using particle in a box model for ideal monatomic gas. Evaluation of rotational, vibrational, electronic and nuclear partition functions. Partition function of monatomic crystal. *Marks 9*

Unit III

Rotational and vibrational entropy of gases, Residual entropy, Free energy and partition functions. General expression for partition function and equilibrium constant. Energy and heat capacity of gasses. Einstein and Debye's theory of heat capacity of solids. *Marks 8*

Unit IV

Calculation of energy and Entropy, heat capacity of polyatomic molecules CO_2, SO_2 etc. Numerical calculations of thermodynamics functions for diatomic and polyatomic molecules.

Marks 8

Recommended books:

1. Physical Chemistry by P.W. Atkins
2. Physical Chemistry by I. N. Levine
3. Thermodynamics for Chemist by S. Glasstone
4. Non Equilibrium Thermodymacis: Principles and application – C. Kalidas & M.V. Sangaranarayanan
5. Non Equilibrium Thermodymacis by de Groot, S. R. and P. Mazur

6. Introduction to Thermodynamics of Irreversible Processes by I. Prigogine
7. Statistical Thermodynamics – M.C. Gupta, Wiley Eastern Ltd.
8. Statistical Mechanics and its Chemical Applications – M. H. Everdell Academic Press.
9. Statistical Thermodynamics – B.J. McClelland, Chapman and Hall Ltd.
10. Fundamental of Statistical Thermodynamic – R.E. Sontagg & Gordon J.V.

Course: 10400
Quantum Chemistry
Credit 3

Total Marks 75 (End Semester 45 + Internal Assessment 30)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**0**	**0**	**3**

Unit I

Review of the basic principles of Quantum Mechanics: Postulates, Hermitian operators, commutation relation. Free particle and particle in a box (One and three dimensional), degeneracy. *Marks 7*

Unit II

Model Systems: Simple Harmonic Oscillator-Schrodinger equation and its solution, Hermite polynomials, two-particle rigid rotor- rotational energy levels of diatomic molecules, particle in a ring, quantum mechanical tunneling. *Marks 10*

Unit III

Hydrogen atom- Schrodinger equation, separation of relative coordinates, radial solution, probability and radial distribution function, angular solution, representation of orbitals, degeneracy, orbital and spin angular momentum. *Marks 10*

Unit IV

Approximate methods: Variation theorem, Linear variation functions. Time independent Perturbation theory for non-degenerate systems (up to second order in energy); application to the helium atom. Hellmann-Feynmann theorem. *Marks 8*

Unit V

Antisymmetry Principle, Slater determinant, Term symbol, spectroscopic states. *Marks 5*

Unit VI

Huckel molecular orbital theory: Postulates, application to ethylene, butadiene, and benzene. Introduction to extended Huckel theory. *Marks 5*

Recommended Books

1. Quantum Chemistry, by Ira N. Levine, Pentice Hall
2. Introduction to Quantum Chemistry by A.K. Chandra, Tata McGraw Hill.
3. Quantum Mechanics by R.K. Prasad, New Age International Publishers, Guwahati

4. Molecular Quantum Mechanics by P.W. Atkins & R.S. Friedman, Oxford University Press.
5. Quantum Chemistry, by D. A. McQuarrie, Viva Books Pvt. Ltd.: New Delhi

Course: 10500
Spectroscopy I
Credit 3

Total Marks 75 (End Semester 45 + Internal Assessment 30)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**0**	**0**	**3**

Unit I:

Electromagnetic spectrum, Interaction of emr with matter, Natural line width and Broadening-Intensity of spectral transitions.

Rotational (microwave) spectroscopy: Classification of molecules according to their moments of inertia, rotational energy levels of HCl, Selection rule for Microwave spectra, intensity, effect of substitution in Microwave spectra. Stark effect, spectra of symmetric top and asymmetric top type molecules. *Marks-9*

Unit II:

Quantum theory of Raman effect, Selection rules, mutual exclusion principle, vibration-rotation Raman spectra. Intensity of Raman lines. *Marks 4*

Unit III:

Fundamental vibrational frequencies, Selection rules and vibrational energy for harmonic and anharmonic oscillators, vibration rotational spectra of diatomic molecules, Fundamental, overtone and combination bands, P, Q and R branches, hot bands, group frequencies, normal modes of vibrations, symmetry of vibrations. *Marks 10*

Unit IV:

Introduction to Photoelectron Spectroscopy : Auger electron spectroscopy *Marks-4*

Unit V:

Chemical shift, factors affecting chemical shift, spin- spin interaction, Coupling constant and Factors affecting, relaxation processes, NOE, Nuclear magnetic double resonance, shift resonance, spin tickling; Proton and ^{13}C NMR spectroscopy of simple organic molecules, living systems – MRI, : Two dimensional NMR, NOESY, DEPT, INEPT terminology, Instrumentation, FT NMR. *Marks-12*

Unit VI:

Electronic spectroscopy: Electronic transitions and selection rules, Frank Condon principle and electronic spectra of polyatomic molecules, Luminescence: Fluorescence and

phosphorescence, solvent effects, absorption and intensity shifts, Calculation of absorption maxima by Woodward-Fieser Rules. *Marks 6*

Text Books :

1. Fundamentals of Molecular Spectroscopy by C.N. Banwell and E.M. McCash, Tata McGraw Hill.
2. Introduction to Molecular Spectroscopy by G.M. Barrow, McGraw Hill.
3. Introduction to Spectroscopy by Donald Pavia, Gary Lampman, George Kriz and James Vyvyan, International student edition
4. NMR in Chemistry, A multinuclear Introduction – William Kemp.
5. Spectrometric Identification of Organic Compounds by R.M. Silverstein, John Wiley.

Reference Book :

1. Spectroscopy – Vol I, Vol II, Vol III edited by B.P. Straughan and S. Walker. Chapman & Hall.
2. Vibrational Spectroscopy – By D.N. Sathyanarayana, New Age International Publishers.

Course 10600 : Practical
Credit - 6

Marks - 150 (End Semester 90 + Internal Assessment 60)	**L**	**T**	**P**	**C**
Time: 18 hours	**0**	**0**	**6**	**6**

Group I. Inorganic Lab **Marks: 25**

Preparation and characterization (viz. conductivity measurement, IR, UV-Vis) of the following complexes:

1. Sodium ferrioxalate, $Na_3[Fe(C_2O_4)_3]\ 9H_2O$
2. Potassium chromioxalate, $K_3[Cr(C_2O_4)_3]$
3. Reinecke's salt
4. Tris-(thiourea) copper(I) sulphate, $[Cu(tu)_3]2SO_4.2H_2O$
5. Tetraamine Cu(II)sulphate, $[Cu(NH_3)_4]SO_4.H_2O$
6. Hexa-amine Ni(II) chloride $[Ni(NH_3)_6]Cl_2$

Group II. Organic Lab **Marks: 25**

Systematic qualitative analysis of organic compounds – Separation and identification of organic compounds from two component mixtures, each having more than one functional group.

Group III. Physical Lab **Marks: 25**

1. To determine the rate constant of hydrolysis of methyl acetate catalyzed by an acid and also the energy of activation.
2. To determine the velocity constant of hydrolysis of ethyl acetate by NaOH.
3. Determine the rate constant of inversion of cane sugar by analytical method.

4. Study the kinetics of the reaction between iodine and acetone in acidic medium by half-life period method and determine the order with respect to iodine and acetone.
5. Determine the molar mass of a polymer by viscometric method.
6. Study the complex formation between Cu^{2+} ion and ammonia by distribution method and find the composition of the complex.
7. To determine the radius of a molecule (glycerol) by viscosity measurements.

IV. Viva-voce *Marks* ***15 (3 × 5 = 15)***
V. Internal Assessment *Marks* ***60 (3 × 20 = 60)***

SEMESTER II

Course 20100
Chemistry of Transition metals and Materials Chemistry
Credit - 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit I: Properties of transition metal complexes:

Transition metals and periodic properties. Transition metal donor-acceptor compounds, Coordination number and geometries, 18-electron rule, Stability of metal complexes, common ligands and complexes, Stereochemically non-rigid systems.

Metal ligand bonding: Ionic surrounding: Crystal Field Theory; Covalent surrounding : Transition metal MO and ligand field Theory, Transition metal complexes with π-bonding ligands.

Molecular orbital model, General view of ML_6 and ML_4 structures: $ML_6(O_h)$, $ML_4(D_{4h})$ and $ML_4(T_d)$, The Angular overlap model (Qualitative) Jahn-Teller Distortion from O_h geometry.

Marks 12

Unit II: Electronic spectra and magnetic properties of transition metals complexes:

Electronic states and terms for transition metals. Selection rules Orgel diagram and Tanabe Sugano diagrams: Application in transition metal electronic spectroscopy. Electronic spectra and structure, d-d and charge transfer transitions, magnetochemistry of transition metal complexes. *Marks 12*

Unit III: Chemistry of Lanthanides and Actinides**:** Electronic configuration, lanthanide contraction, separation of lanthanides, Magnetic and spectral properties of lanthanides, lanthanide shift reagents. *Marks 8*

Unit IV: Photochemical reactions of Transition metals:

Basic photochemical processes, photosubstitution reactions, photoredox reactions, ligand photoreactions, photoreactions and solar energy conversion. *Marks 8*

Unit V: Solid state reaction:

General principle, experimental procedure, coprecipitation as precursor, kinetics of solid state reactions. Crystallization, melts, glasses and gels. Zeolite synthesis and applications.*Marks 6*

Unit VI: Graphite and zirconium intercalation compounds, transition metal dichalcogenide. Preparation of thin films, growth of single crystals. Catalyst immobilization onto silica and clay surfaces and applications, pillaring of certain clays.. Electronic and optical properties of some inorganic and organic solids. Design and properties of composites, polymer matrix and carbon-carbon composites. Clay and ceramic composites, Brief idea about drilling muds.

Marks 14

Recommended Books:

1. Inorganic Chemistry, W.W. Porterfield, 2nd Edition, Academic Press
2. Inorganic Chemistry, Shriver & Atkins, 5th Edition Oxford
3. Solid State Chemistry and its applications (2005) A.R. West, John Wiley & Sons
4. Composition & properties of Drilling and completion Fluids, 6th edition, (1995) H.C.H. Darley & G.R. Gray Gulf Publishing Co.
5. Composite Materials, K. Srinivasa, Narosa, 2010
6. Polymer composite, M.C. Gupta & A.P. Gupta. New Age Int. (P) Ltd., 2005

Course-20200
Natural Products and Heterocyclic Chemistry
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**4**	**0**	**0**	**4**

Unit I

Alkaloids : Occurance, classification, general methods of isolation, test for detection. Structure elucidation by physical and chemical methods and synthesis (including retrosynthetic approach) of : Nicotine, Piperine, Papaverine, Atropine and Morphine. *Marks-15*

Unit II

Terpenoids : Occurance and classification, isoprene rule, general methods of isolation. Biogenetic pathway of mono- and sesquiterpenes. Structure determination by physical and chemical methods and synthesis of the following:

Acyclic monoterpenoid – Linalool.

Monocyclic monoterpenoid –α-Terpeneol, Carvone, Metnthol, Piperitone, Pulegone,

Bicyclic monoterpenoid: α-pinene, Camphor, Camphene, borneol. *Marks-15*

Unit III

Carbohydrates : Structure, reaction and conformation of disaccharides – sucrose, maltose and lactose. Polysaccharides – starch and cellulose.

Peptides and Proteins : Structure determination and synthesis of small peptides (di-, tri- and tetra-). Solid phase synthesis of peptides. Classification of proteins. Primary, secondary and tertiary structure of proteins. *Marks-15*

Unit IV

Heterocyclic Chemistry: Nomenclature; π-excessive and π-deficient heterocycles, Principles of heterocyclic synthesis involving cyclization and cyclo-addition reaction.

Synthesis and properties of three, four, five, six and seven membered heterocycles containing one, two and three heteroatoms viz., N, O and S (aziridine, oxirane, thiirane, azetidine, oxetane, thietane, pyrazole, isoxazole, isothiazole, imidazole, oxazole and thiazole, pyran, azepine, oxepine. thiepine). heterocycles. Elementary idea of Click Chemistry. *Marks-15*

Recommended books

Natural products Chemistry:

1. Organic Chemistry of Natural Products, Vol I and II, Gurdeep Chatwal, Himalaya Publishing House, Bombay.
2. Chemistry of Organic Natural Products, Vol I and II , O.P. Agarwal, Goel Publishing House, Meerut.
3. The Alkaloids: K. W. Bentley.
4. Organic Chemistry, Vol- II, I.L. Finar

Heterocyclic Chemistry:

1. Heterocyclic Chemistry : Synthesis, Reactions and Mechanisms – Raj K. Bansal, Wiley Eastern.
2. Heterocyclic Chemistry – T.L. Gilchrist, Longman Scientific and Technical/Pitman Publ. Ltd.

Course: 20300

Physical Chemistry II (Electrochemistry, Surface Chemistry and Solid State Chemistry)

Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Group A

Electrochemistry (Marks 25)

Unit I

Ion-Solvent Interaction: Ion-Dipole, Ion-quadruple, Ion-Induced Dipole Interaction, Ion-Association: Bjerrums hypothesis, Thermodynamics of ion-pairing, relation between Debye-Huckel free ion and Bjerrums ion-pair. *Marks 8*

Unit II

Polarizable and non polarizable electrodes. Inner and Outer potential, Thermodynamics of Electrified Interfaces: Surface Excess and its determination. *Marks 5*

Unit III

Electrical double layer (DL): HP/ GC/ Stern model. Potential variation in DL and capacity of DL. *Marks 7*

Unit IV

Different types of corrosion, mechanism and prevention of corrosion. *Marks-5*

Group B
Surface Chemistry (Marks 25)

Unit I

Adsorption of gases on solid surfaces

Adsorption isotherm, shapes of isotherms, Langmuir's theory and its limitations. Derivation of BET equation. Determination of surface area of an adsorbent, thermodymics of adsorption processes.

Capillary condensation – adsorption in micropores, hysteresis loop. *Marks-6*

Unit II

Kinetics and Mechanism of heterogeneous catalysis–Langmuir-Hinshelwood model, Eley-Riedel model, unimolecular and bimolecular surface reaction, decomposition of ammonia (NH_3).

Chemisorption: Chemisorption on metals, semi-conducting oxides and insulator oxides, electronic theory of chemisorption. *Marks-9*

Unit III

Electrical aspects of surface chemistry, Electro kinetic phenomena, the structure of electrical double layer, Zeta potential and colloidal stability, Measurement of zeta potential.

Surfactants – definition and classification, micelle formation and determination of critical micelle concentration.

Reverse micelle and its application, solubilization, microemulsion. *Marks 10*

Group C
Solid State Chemistry (Marks 10)

Types and structure of solids, brief description of crystal symmetry, Space group (Monoclinic and Triclinic system), line and plane defects, Octahedral and tetrahedral voids, Radius ratio rule. Electronic Structure: Band theory of solids, electrical, optical and magnetic properties of solids. *Marks 10*

Recommended Books

1. Modern Electrochemistry – Vol I, II by J. O. M. Bockris & A. K. N. Reddy

2. Electrochemistry by Glasstone
3. Physical Chemistry by Atkins
4. Chemical Kinetics by K. J. Laidler
5. Physical Chemistry by Adamson
6. Basic Solid State Chemistry by A. R. West
7. Solid State Chemistry: An Introduction by L. E. Smart and E. A. Moore
8. Solid State Chemistry by D. K. Chakravorty
9. New Directions in Solid State Chemistry- C N R Rao and J Gopalakrishnan
10. Principles of Solid State Chemistry by H. V. Keer
11. Comprehensive Physical Chemistry by N. B. Singh, N. S. Gajbhiye and S. S. Das

Course: 20400
Symmetry and Group Theory
Credit – 3

Total Marks - 75 (End Semester 45 + Internal Assessment 30)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**0**	**0**	**3**

Unit-I:

Symmetry operation, elements of symmetry: Matrices and matrix representation of symmetry operations, Definition of Group, finite and infinite group. Examples of groups using geometrical object and symmetry operations. Symmetry elements as elements of group. Point groups. *Marks-10*

Unit II:

Orthogonality theorem: reducible and irreducible representation, use of vectors and mathematical functions in group representation, Character table for molecular point group, construction of C_{2v} and C_{3v} Character table. Direct product representation. Projection operator, symmetry adapted linear combination (SALC) for C_{2v}, C_{3v}, D_{4h} and Td point group molecules.

Marks-15

Unit III:

Chemical Application of Group Theory: Use of group theory in construction of hybrid Orbitals (d^2sp and sp^3 hybrids). Infrared absorption and Raman scattering spectroscopy, vibrational modes as bases for group representation, Symmetry selection rules for IR and Raman Spectra. Classification of vibrational modes and vibrational analysis. Orbital Symmetry and Chemical reactions –Woodward and Hoffman rules for electrocyclic and cycloaddition reactions.

Marks-20

Text books :

1. Chemical Applications of Group Theory by F.A. Cotton, Wiley Intersciences.
2. Symmetry and Spectroscopy of molecules K. Veera Reddy, New-Age International (P) Ltd. Publishers, Guwahati, 2005
3. Group Theory in Chemistry by M.S. Gopinathan; V. Ramakrishnan, Vishal Publishing Co, 2006

Reference books:

1. Vibrational Spectroscopy by D.N. Sathyanarayana, New-Age International Publishers 2005
2. Introductory Group theory for Chemists by George Davidson, Elsevier Publishing Company Ltd., London.

Course: 20500
Spectroscopy II
Credit - 3

Total Marks - 75 (End Semester 45 + Internal Assessment 30)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**0**	**0**	**3**

Unit I:

Mass spectrometry: Ion fragmentation mechanism, Base peak and molecular ion peak, metastable peak, instrumentation and techniques, ionization methods, isotopic distribution, Application in determining the structure of organic and inorganic compounds. *Marks 8*

Unit II:

ESR: Origin of g-value , spin orbit coupling, line shape, Kramer degeneracy Application of ESR in organic radical chemistry and transition metal coordination chemistry. M*arks 8*

Unit III:

Vibrational and electronic spectroscopy in Inorganic compounds:

Symmetry criteria for intensity of spectroscopic transions, symmetry and spectral changes upon coordination.

Infrared and Raman spectroscopy: Symmetry and IR/Raman activity of normal of vibrations, Mutual exclusion principle, interpretation of IR and Raman spectra of simple organic and inorganic compounds. *Marks 9*

Unit IV:

Spectroscopic methods in analysis of molecular composition/Structure: Use of IR, electronic, ^{1}H, ^{13}C & ^{31}P NMR, Mass spectrometry. *Marks 20*

Recommended books –

1. Fundamentals of Molecular Spectroscopy: C.N. Banwell and E.M. McCash, Tata McGraw Hills
2. Introduction to Spectroscopy by Donald Pavia, Gary Lampman, George Kriz and James Vyvyan, International student edition.
3. Spectroscopic Methods in Organic Chemistry – D.H. Williams and I. Fleming
4. NMR in Chemistry : A Multinuclear Introduction – William Kemp, Macmillan
5. Spectrometric Identification of Organic Compounds - Silverstein, Webster and Kiemle, Wiley.

Course 20600
Laboratory Course
Credit - 6

Total Marks - 150 (End Semester 90 + Internal Assessment 60)	**L**	**T**	**P**	**C**
Time – 18 hours	**0**	**0**	**6**	**6**

Group I. Inorganic Lab **Marks: 25**

A. Preparation and characterization (viz. equivalent conductance measurement, IR, UV-Vis) of the following complexes

1. Potassium chromithiocyanate
2. Sodium Cobaltinitrite $Na_3[Co(NO_2)_6]$
3. Chloropentamine Cobalt (III) chloride $[Co(NH_3)_5Cl]Cl_2$
4. Nitropentamine Cobalt(III) chloride $[Co(NO_2)(NH_3)_5]Cl_2$
5. Nitrito Pentamine Cobalt(III) chloride, $[Co(ONO)(NH_3)_5]Cl_2$

B. Analysis

1. Estimation of Mg^{2+} and Ca^{2+} by complexometric method in different ores with one / two components.
2. Analysis of amount of Zn^{2+}, Cu^{2+} ions in a given solution

Group II. Organic Lab **Marks: 25**

1. Organic Estimation -
   i) Estimation of glucose and sucrose in a mixture.
   ii) Estimation of acetone by iodoform method.
   iii) Estimation of hydroxyl and amino groups by acetylation method.
2. Separation and identification of three components of organic compounds present in a mixture by TLC.

Group III. Physical Lab **Marks: 25**

1. To study hydrolysis of methyl acetate in presence of HCl and H_2SO_4 and hence determine the relative strength of the acids (Guggenheim method).
2. To study the inversion of cane sugar in presence of HCl and H_2SO_4 and hence determine the relative strength of the acids by polarimeter (Guggenheim method).
3. To study the kinetics of reaction between $K_2S_2O_8$ and KI.
   (a) Determine the rate constant and order of the reaction
   (b) Study the influence of ionic strength on the rate constant.
4. Determine the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method.
5. Determine the relative strength of acetic acid and monochloro acetic acid by conductance measurement.
6. Determine the specific rotation of sucrose and hence determine the unknown concentration of supplied solution by polarimetric measurements.
7. Determination of pH of a mixture of CH_3COOH and CH_3COONa, and hence determine the dissociation constant of the acid.

IV. Viva-voce *Marks **15 (3 × 5 = 15)***

V. Internal Assessment *Marks **60 (3 × 20 = 60)***

SEMESTER III

Course-30100
Advanced Inorganic Chemistry
Credit -4

Total Marks - 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit-I : Transition metal donor acceptor compounds and reaction mechanism.

(A) Lability and inertness, stability constant- formation constant of complexes in solutions, mechanism of ligand replacement reactions: Substitution reactions in octahedral and square planar planer complex., trans effect and its importance, idea concerning electro transfer reactions, inner and outer sphere reactions. *Marks 10*

(B) Introduction to transition metal organometallic chemistry: Metal carbon bond formation, Role of Pauling electronegativity of metal, μ and ή- notation, electron counting rules, number of electron donated by various ligands; 18 electron rule- MO description and limitations. Isolobel analogy and organometallic compounds. Bonding in organotransition metal compounds: Metal carbonyls, metal olefins, metal carbone, Role of co-ligands like phosphine, arsine, stibine, N_2, O_2 and NO. Oxidative addition, reductive elimination and β-elimination reaction. *Marks 10*

Unit-II

(A) **Application of NMR spectroscopy** (^{1}H, ^{31}P and ^{19}F) : Chemical shift, factors contributing to chemical shift, spin-spin coupling and its implication to structure determination; simplification of complex spectra; Use of ^{31}P and ^{19}F NMR in coordination chemistry: metal-ligand interaction; isomer determination; evaluation of stereo chemical non-rigidity in molecules; NMR spectra of paramagnetic compounds. *Marks 08*

(B) **ESR spectroscopy**: Principle, resonance condition, Hyperfine & superhyper interaction, line width, zero-field splitting and application to d^1, d^3 and d^9 complexes. *Marks 08*

(C) **Mossbauer spectroscopy**: Principle of Mossbauer spectroscopy, Instrumentation, Application of Mossbauer spectroscopy: the isomer shift, magnetic interaction, quadruple splitting, line with. Application to iron to iron and tin compounds. *Marks 08*

(D) **NQR spectroscopy**: Principle of NQR, Quadruple constant, Application of NQR spectroscopy. *Marks 06*

Unit-III : **Magnetochemistry**

Types of magnetic bodies (eg, Diamagnetic, Paramagnetic, ferromagnetic and antiferro magnetic), antiferromagnetic coupling, Magnetic properties based on crystal field theory:

spin only magnetic moments, spin-state equilibrium in octahedral stereochemistry: cross-over region, quenching of orbital magnetic moment by CF, orbital contribution, effect of temperature on magnetic behaviour, magnetic properties of octahedral, tetrahedral, tetragonally distorted octahedral and sequence planer complexes. Experimental determination of magnetic susceptibility: Gouy's and NMR methods.

L-8, Marks – 10

Course: 30200
Advanced Organic Chemistry
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40) **L T P C**
Time: 3 hours **3 1 0 4**

Unit I : Stereochemistry

Conformational analysis of disubstituted cyclohexanes, cyclohexene, cyclohexanone, 2-alkyl, 3-alkyl, and 4-alkyl ketone effects. $A^{1,2}$ and $A^{1,3}$ strains. Conformation of fused systems – decalins and perhydrophenanthrenes. Effects of conformation on reactivity and mechanism of basic organic reactions of 6-membered ring compounds. Marks-10

Chiroptical properties – Optical rotatory dispersion, circular birefringence, circular dichroism, axial haloketone rule, octane rule. Marks-5

Unit II : Organic synthesis I

Organometallic reagents in formation of carbon-carbon bonds: Organopalladium in C-C formation (Heck reaction, Stille, Suzuki, Sonogashira and Negishi Coupling).

Formation of C=C bonds by elimination reactions, syn elimination; Wittig and related reactions, McMurry reaction, Peterson olefination, Julia reaction and Tebbe olefination.

Use of organosulphur compounds for reversal of polarity (Corey-Seebach Umpolung).

Allylic activation by π-allyl Ni and π-allyl Pd complexes. Marks-15

Unit III: Organic synthesis II

Definition and Classification. Oxidation by Mn(VII) and Cr(IV) reagents.

Oxidation (i) of carbon-carbon double bond : dihydroxylation by $KMnO_4$, OsO_4 (including Sharpless asymmetric dihydroxylation), iodine and silver carboxylate (Woodward and Prevost condition) and peroxy acid. Allylic and benzylic oxidation of alkene : Use of SeO_2 and DDQ.

(ii) of alcohols : Use of Cr(VI) based reagents (PCC, PDC), DMSO-based reagents (Swern, Pfitzner-Moffatt and Albright – Goldman), Tetrapropyl ammonium perruthenate (TPAP);

(iii) of 1,2- diols.

Reduction (i) by catalytic hydrogenation : both heterogeneous (H_2/Pd-C, H_2/Pt_2O, Lindler's and Rosendmund's reduction) and homogeneous (Wilkinson catalyst), (ii) by hydride transfer ($LiAlH_4$, Lithium trialkoxy aluminium hydrides, $LiBH_4$, DIBAL, $NaBH_4$, $NaCNBH_4$, SMEAH (Red Al), Superhydride and selectrides, 9-BBN (iii) by dissolving metal (alkali metals in liquid ammonia) and (iv) by diimide.

Electrooxidation and reduction, Use of Baker's Yeast. Marks-20

Unit IV: Organic synthesis III :

Application of Enamines, Hydroboration and trialkylsilyl halides in organic synthesis.

Use of the following reagents: Organotin (TBTH), Lithium Diisopropyl Amide (LDA), Dicyclohexyl carbodiimide, Dicyanodichloroquinone (DDQ), Dimethyl dioxirane (DDO), lipase. Marks-10

Recommended Books

Stereochemistry :

1. Stereochemistry of Organic Compounds – D. Nasipuri, Wiley Eastern
2. Stereochemistry of Carbon Compounds – Earnest E. Eliel, Tata McGraw Hill
3. Stereochemistry of Carbon Compounds – Subrata Sengupta, New Central Book agency, Kolkata
4. Stereochemistry and Mechanism through Solved Problems- P.S. Kalsi, New Age International Publishers

Organic Synthesis :

1. Modern Methods of Organic Synthesis – Carruthers and Mendham, Cambridge University Press
2. Organic Synthesis – M.B. Smith, McGraw Hill. (Reference book)
3. Principles of Organic Synthesis – R.O.C. Norman and J M Coxon
4. Advanced Organic Chemistry Part A and B : Carey and Sundberg
5. Organic Synthesis – J. Singh and L.D.S.Yadav, Pragati Prakashan
6. Application of Redox and Reagents in Organic Synthesis- R.K. Kar, New Central Book Agency
7. Fundamentals of Organic Synthesis : The Retrosynthetic Analysis - R.K. Kar, NCBA
8. Synthetic Approaches in Organic Chemistry – R.K. Bansal- Narosa Publishing House, New Delhi
9. Modern Synthetic Reactions – H.O. House, W.A. Benjamin, NY

Course: 30300

Physical Chemistry III

(Chemical Dynamics, Polymer Chemistry and Photochemistry)

Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Group A

Chemical Dynamics (Marks 25)

Methods of determining rate laws, Activated complex theory, structure of transition state, Erying equation, chain reactions and oscillatory reaction, steady state approximation.

Unimolecular reactions – Drawbacks of Lindemann theory, Hinshelwood, Kassel, Rice and Ramsperger theory, Stater's Theory.

Relaxation kinetics – linearized rate equation, relaxation time (in single step reaction) ; determination of relaxation time and rate constant, Methods of studying fast reaction – flow method, temperature jump and pressure jump method, NMR method.

Reactions in solution – Factors determining reaction rates in solution, reactions involving ion-ion and ion-dipoles reaction; influence of solvent, ionic strength and pressure on the reactions in solution.

Rate of enzyme catalyst reaction, Michaelis-Menten equation; temperature, pH and concentration dependence of enzyme catalysed reactions; acid-base catalysis and acidity function. *Marks 25*

Group B

Polymer Chemistry (Marks 25)

Condensation polymerization: Chemistry and kinetics, Coarother's equation.

Free radical polymerization: Chemistry and steady state kinetics, cage effect, chain transfer reactions, Mayo equation and evaluation of chain transfer constant, inhibition and retardation, allylic polymerization and auto-inhibition.

Nonradical chain polymerization: Cationic and anionic polymerization–Chemistry, Kinetics and degree of polymerizations. Living polymers.

Copolymerization: types of copolymerization, technical importance of copolymerization. copolymerization equation, monomer reactivity ratio, its determination.

Polymer degradation: Thermal degradation, radiation induced degradation, oxidative degradation, antioxidant. *Marks 25*

Group C

Photochemistry (Marks 10)

Concept of quantum yield and its determination; Fluorescence emission and structure; Triplet state and phosphorescence emission; delayed fluorescence; Photochemical primary process –

classification of photochemical reactions; rate constant and life-times of reactive species; types of photochemical reactions–photodissociation, photoisomerisation (cis-trans).; photogalvanic cell

Recommended Books

1. Chemical Kinetics – K.J. Laidler
2. Theories of Chemical Kinetics – Laidler, Glasstone , Erying
3. Kinetics and Mechanism – Frost and Pearson.
4. Polymer Science by V.R. Gowarikar, N. V. Viswanathan and Jayadev Sreedhar
5. Polymer Science and Technology of Plastics and Rubbers – Premamoy Ghosh
6. Introduction to Polymer by R. J. Young and P. A. Lovell
7. Fundamentals of Photochemistry by Rohatgi-Mukherjee
8. Photochemistry by Calverts and Pitts

Course: 30400
Advanced Topics in Chemistry
Credit 3

Total Marks 75 (End Semester 45 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 2.5 hours	**3**	**0**	**0**	**3**

Unit I: Computational Chemistry Marks-15

Representation of molecules: Cartesian and Internal Assesment Coordinates; Geometry Optimization (Newton-Raphson), vibrational frequencies; ionization potential and electron affinities of molecules. BO approximation, potential energy surface, SCF theory, Gaussian basis sets, Basic idea of Molecular Mechanics and force field; Molecular dynamics: basic concept, Verlet and Velocity-Verlat algorithm; Basic ideas of structure activity relationship. Introduction to popular softwares (like Gaussian, GAMESS).

Unit II: Bio-Chemistry Marks-15

Enzymes and Co-enzymes : Classification of enzymes; Chemical nature of enzyme, Specificity of enzyme, Mechanism of enzyme action, Factors effecting enzyme action, Michaelis Menten Equation, Double reciprocal plot. Mechanism of action of chymotrypsin.

Co-enzymes, co-factors, prosthetic groups: Mechanism of action of NAD^+, $NADP^+$, FMN, FAD. Functions of ATP.

Nucleic acids: Review on chemical constitution and biological role of nucleic acids. Double heical structure of DNA. Chemical basis of heredity, Genetic code, Replication of DNA. Transcription and translation.

Unit III: Supramolecular Chemistry Marks-15

Introduction to Supramolecular Chemistry, Concepts of host guest chemistry, classification, thermodynamics and kinetic stability, Non-covalent interactions, Molecular recognition,

Recognition of anionic substrates, Supramolecular reactivity and catalysis, Effects of medium, Chiral recognition and catalysis.

Molecular receptors for different types of molecules: Crown ethers, cryptands, cyclodextrins, Calixarenes

Molecular devices: ionic, electronic and switching devices

Books Recommended:

Computational Chemistry:

1. Introduction to Computational Chemistry by Frank Jensen
2. Essentials of Computational Chemistry: Theories and Models by C. J. Cramer
3. Molecular Modeling: Principles and Applications by A. R. Leach
4. Computational Chemistry Workbook by T. Heine, J-O. Joswig and A. Gelessus

Biochemistry:

1. Principles of Biochemistry – A.L. Lehninger, D.L. Nelson and M.N. Cox, CBS Publishers and Distributors
2. Outlines of Biochemistry – E.E. Cohn and Stampf, Wiley Eastern
3. Harper's Biochemistry.
4. Textbook of Biochemistry : U Satyanarayana.

Supramolecular Chemistry:

1. Supramolecular Chemistry: Concepts and Perspectives- Jean M. Lehn, VCH
2. Supramolecular Chemistry – Paul D. Beer, Philip A. Gale and David K. Smith; (Oxford Chemistry Primer)

Course: 30500
Petrochemical Process Technology
Credit 2

Total Marks 50 (End Semester 30 + Internal Assessment 20)	**L**	**T**	**P**	**C**
Time: 2 hours	**2**	**0**	**0**	**2**

(Field visit to Brahmaputra Gas Cracker Ltd, Assam Petrochemicals Ltd, Digboi Refinery etc. as a part of Internal Assesment Assessment)

Unit I Marks-10

Petrochemical feedstock in India (Petroleum fractions, natural gas, tertiary recycling, pyrolysis gasoline); Petrochemical product profile (Polymers, synthetic fibre, synthetic rubber, detergent, intermediates).

Physico-chemical properties of hydrocarbons, crude oil evaluation, crude quality and pretreatment of crude oils, natural gas processing, petroleum refining process, sulphur recovery, petroleum products.

Unit II Marks-5

Steam cracking for production of olefins, steam cracking process technology – Hot section, cracked gas compression & dehydration, operating variables in steam cracking,

thermal cracking reactions, coke formation, decoking in thermal cracker, emerging technologies for olefins production.

Unit III Marks-10

Reactions in catalytic reforming, reforming catalysts, process variables in catalytic reforming, aromatic extraction & separation, dearomatizing of naphtha, aromatic conversion processes – disproportionation of toluene, hydroalkylation and isomerization. Synthesis gas and ammonia production, urea production, synthesis gas process technology, CO, Fischer-Tropsch Syngas technology, methanol, formaldehyde and acetic acid production. Ethylene and ethylene derivatives, propylene and its derivatives.

Unit IV Marks-5

Environment management and corrosion prevention in petrochemical process industries including production and quality of DM water.

Books Recommended:

Petrochemical Process Technology by I. D. Mall

Course 30600
Laboratory Course
Credit – 6

Total Marks - 150 (End Semester 90 + Internal Assessment 60)	**L**	**T**	**P**	**C**
Time: 18 hours	**0**	**0**	**6**	**6**

Group I. Inorganic Lab **Marks: 25**

Analysis

1. Estimation of Zn^{2+} and Ni^{2+} by complexometric and Fe^{2+}, Mn^{2+}, Ni^{2+} by colorimetric method in different ores with one / two components.
2. Estimation of alloys – Brass, Bronze
3. Complete analysis of water
4. Analysis of soil samples (pH, Fe^{3+}, Ca^{2+}, Na^{+}, K^{+}, organic matter, porosity and clay content).

Group II. Organic Lab **Marks: 25**

1. Separation and identification of amino acids present in a mixture by paper chromatography.
2. Organic Preparation -

One –step preparation

i) Cannizaro reaction of benzaldehyde (separation of benzyl alcohol and benzoic acid by solvent extraction)

ii) Oxidation of p-nitrotoluene to p-nitrobenzoic acid

iii) Reduction of benzophenone to benzhydrol

iv) Phthalic anhydride to phthalimide

Two –step preparation

i) p-nitrobenzene azo 2-naphthol (Para Red) from p-nitroaniline

ii) Benzanilide from benzophenone

iii) Dibenzyl from benzoin

Group III. Physical Lab **Marks: 25**

1. Determination of hydrolysis constant of aniline hydrochloride by pH measurements.
2. Determine the strengths of the components of the following mixtures by conductometric titration
   (a) Hydrochloric acid and acetic acid
   (b) Sulphuric acid and copper sulphate
3. Determine the strengths of HCl and CH_3COOH in a given mixtures by pH-metric titration.
4. Verify Beer's law and determine the unknown concentration of supplied solutions like $KMnO_4$ / $K_2Cr_2O_7$
5. Determine the composition of iron-salicylic acid complex spectrophotometrically by Job's method.
6. Determine the partial molar volume of ethanol by determining the densities of dilute aqueous solutions.
7. Perform theoretical calculations using a computer
   (a) Least squares fitting and plotting linear and exponential graphs.
   (b) Charge density distribution and shapes of s and p orbitals.
   (c) Potential energy diagram of hydrogen molecule ion

IV. Viva-voce *Marks* ***15 (3 × 5 = 15)***

V. Internal Assessment *Marks* ***60 (3 × 20 = 60)***

SEMESTER IV

Course 40100
Physical Methods in Chemical Analysis
Credit–3

Total Marks: 75 (End Semester 45 + Internal Assessment 30)	**L**	**T**	**P**	**C**
Time: 2½ hours	**3**	**0**	**0**	**3**

Unit I: Principles and applications of powder and single crystal XRD. *Marks 10*

Unit II: *Marks 5*

Polarography, Basic principles, instrumentation and applications of cyclic voltammetry

Unit III: *Marks 10*

Thermal methods: Principles and applications of thermogravimetry (TG), Derivative thermogravimetry (DTG), Differential thermal analysis (DTA) and Differential scanning calorimetry (DSC).

Unit IV : *Marks 10*

Chromatographic methods: Adsorption, liquid-liquid partition, ion–exchange, HPLC, gel permeation chromatography and gas chromatography, HPTLC, Flash chromatography.

Unit V: *Marks 10*

Transmission electron microscopy (TEM) and scanning electron microscopy (SEM), AFM

Recommended books –

1. Instrumental Methods of Chemical Analysis - H Kaur, Pragati Prakashan
2. Introduction to Thermal Analysis: Techniques and Applications- M.E. Brown, Springer
3. Introduction to Instrumental analysis – R.D. Braun, McGraw Hill.

Course 40200
Introduction to Green Chemistry
Credit – 1

Total Marks - 25 (End Semester 15 + Internal Assessment 10)	**L**	**T**	**P**	**C**
Time: 1 hour	**1**	**0**	**0**	**1**

Evolution of Green Chemistry-the background, Tools of green chemistry, Principles of green chemistry. Concept of Atom Economy. Green starting materials, Green reagents, Green solvents (Water, Ionic liquid, Polyethyle glycol, Super Critical Fluids etc), Green reaction conditions and Green chemical products. *Marks 15*

Recommended Books :

Principles of Green Chemistry : Paul Anastas and J Werner
Green Chemistry : V.K. Ahluwalia

Course 40300
Research Methodology

Credit – 1

Total Marks - 25 (End Semester 15 + Internal Assessment 10)	**L**	**T**	**P**	**C**
Time: 1 hour	**1**	**0**	**0**	**1**

Research Methodology:

Introduction, Finding a suitable research topic, review of literatures, Aim and Objective of research, Materials and methods, Collection of data, Results and discussions, how to conclude the discussions. Reference writing. Impressive presentation. Brief idea about online submission to journals, dissertation and thesis writing, citations and impact factors of journals.

Marks 15

Recommended Books : Research Methodology: Methods and Techniques by C. R. Kothari

Course 40410 : Elective I
Inorganic reaction mechanism and kinetics
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit I

Formation constants, chelate effect, Thermodynamic and Kinetic stability; inert and labile complexes; Stability constant; Correlation of stability constant with thermodynamic factors – G,H and S. Factor affecting thermodynamic stability; Determination of stability constant – Jobs and Bjerrum's methods. *Marks 12*

Unit II

Mechanism of ligand replacement reactions; Factor affecting the rate of substitution reaction; Substitution reaction in square planner complexes [Rh(I), Pt(II) and Pd(II)] complexes; Trans effect and its applications; Substitution reactions in octahedral complexes [Cr(III), Co(III)]; Rate of water replacement reaction; Solvolysis and hydrolysis reaction; acid hydrolysis and base hydrolysis reaction; Synthesis of coordination compound by substitution reactions; Isomerization and racemization of tris-chelate complexes; Molecular rearrangement in four-coordinated and six-coordinated complex. *Marks 26*

Unit III

Idea concerning electron transfer reaction: Inner sphere reaction; outer sphere reaction; Rearrangement of Precursor complex and electron transfer; Nature of bridging ligand; 2-electron transfer; Synthesis of coordination compounds using redox reaction;

complementary and non conplementary reaction; Oscillating reactions; Template effect and macrocyclic ligands; reactions of coordinated ligands. *Marks 22*

Recommended Text Books

1. Inorganic Chemistry: Principles of structure and reactivity, 4th Edition; J.E. Huheey, E.A. Keiter, R.L. Keiter, O.K. Medhi,
2. Advanced Inorganic Chemistry, 6th Edition, F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann.
3. Inorganic Chemistry, K.F. Purcell and J.C. Kotz.

Course 40420 : Elective I
Organic Synthesis
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit I

Pericyclic reactions – Classification of pericyclic reactions, FMO method, Orbital symmetry correlation method, PMO method for the explanation of pericyclic reactions under thermal and photochemical conditions; Cycloaddition reactions: [2+2], [4+2], [6+4] cycloadditions, 1,3-dipolar cycloadditions; the ene reaction, cheletropic reactions, Sigmatropic rearrangement – [m+n] sigmatropic shifts of hydrogen and carbon, Cope and Claisen rearrangement. Electrocyclic reactions, Stereoselectivity and regioselectivity of pericyclic reactions. *Marks-20*

Unit II

Photochemistry of organic compounds – Photochemical energy, Jablonski diagram, photosensitization, quenching.

Olefinic photochemistry – Photostereomutation of cis-trans isomers, optical pumping, [2+2] cycloadditions, photochemistry of conjugated dienes – cycloaddition and dimerisation of butadiene, photochemistry of vision.

Photochemistry of carbonyl compounds – Norrish type I and type II processes, photoreduction of saturated aryl alkyl and α,β-unsaturated ketones, Paterno-Buchi reaction, Photorearrangements – di-π-methane rearrangement and rearrangement of cyclohexadienes, Reaction of singlet, oxygen, photooxidation. *Marks-20*

Unit III

Elementary idea of PASE synthesis, Combinatorial Chemistry, Parallel synthesis, Microwave synthesis. Nanocatalysis in Organic synthesis. Olefin metathesis.

Study of the following reactions, their mechanism and synthetic utility

Henry reaction, Mitsunobu reaction, Corey-Nicolaou macrolactonization, Baylis Hilman reaction, Vilsmeier–Haack reaction, Sharpless asymmetric epoxidation, dihydroxylatioin and aminohydroxylation, Wohl Ziegler allylic bromination, Barton reaction. *Marks-20*

Recommended Books

Pericyclic Reactions :

1. Frontier Orbitals and Organic Chemical Reaction – Ian Flaming, John Wiley
2. Advanced Organic Chemistry Part A and B - Carey and Sundberg

Organic Photochemistry :

1. Organic Photochemistry – J.M. Coxton and B. Halton, Cambridge University Press.
2. Introductory Photochemistry – A. Cox and T.J. Kemp, McGraw Hill
3. Elements of organic photochemistry – Dwaine O. Cown and Ronald L. Driske, Plenum Press, New York and London
4. Photochemistry and Pericyclic Reactions : J Singh and J Singh, New Age International Publishers
5. Fundamentals of Photochemistry – K.K. Rohatgi-Mukherji, Wiley Eastern

Organic Synthesis:

Same as given for Course 30200

Course 40430 : Elective I
Advanced Polymer Chemistry
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit I

Polymerization processes: Step polymerization, chain polymerization including carbonyl polymerization, Ziegler–Natta co-ordination polymerization, atom transfer free radical polymerization, supramolecular polymerization, ring opening polymerization, metathesis polymerization, group transfer polymerization. *Marks-12*

Unit II

Copolymerization: Step copolymerization, chain copolymerization, Types of copolymers, Copolymer equation, Monomer reactivity ratios. Structure and reactivity of monomers and radicals, Alfrey price Q-e scheme, Block and graft copolymers. *Marks 18*

Unit III

Polymer characterization: Average molecular weight concept, Number average, weight average, viscosity average molecular weights. Polydipersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group analysis, viscosity, light scattering, osmotic and ultrantracentrifugation methods, fractionation of polymers, molecular weight distribution, GPC. Chemical analysis of polymers:

Spectroscopic methods, X-ray diffraction study, microscopy, thermal analysis, thermal transition in polymer (Tg, Tm). *Marks 20*

Unit IV

Polymer in Special uses: High temperature and fire resistant polymers, Liquid crystal polymers, Conducting polymers, polyelectrolytes, degradable polymers. *Marks 10*

Recommended books

1. Principle of Polymerization – George Odian,John Wiley & Sons. INR
2. Introduction to Polymers – R.J. Young and P.A. Lovell, Nelson Thornes Ltd.
3. Macromolecules, an introduction to Polymer Sciences, edited by F.A. Bovey & F.H. Winslow, Academic Press.
4. Analysis and Characterization of Polymers, edited by Sukumar Maiti, Anusandhan Prakashan.
5. Polymer Chemistry: An Introduction by M. P. Stevens, Oxford University Press.

Course 40510: Elective II
Transition Metal Organometallics and Metal Clusters
Credit – 4

Total Marks -100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit I

Transition metal organometallics: Organization of organometallic Chemistry and historical developments. Carbon σ donors: Synthesis of metal alkyls and aryls, direct reaction of a metal with organic halides, reaction of anionic alkylating agents with metal halides. Metallation reactions, Hydrometallation, Oxymetallations and Halometallations. Structure and bonding in metal alkyls and aryls. Synthesis, properties, structure and bonding in metal carbonyl carbon π donors : Synthesis, structure and bonding in olefins, acetylane, butadiene, cyclobutadine and π-allyl metal complexes. Structure and bonding in arene metal complexes, 16 and 18-electron rules.

Reactions of organometallic compounds: Oxidative addition and reductive elimination reactions. Catalysis by organometallic compounds, hydrogenation, hydroformylation, oligomenization and polymerizations.

Activation of small molecules (O_2, H_2, CO and CO_2). *Marks 40*

Unit II

Clusters (including C_{60} and boronhydrides)

Definition of clusters, Low and high nuclearity metal carbonyl and metal halide clusters, their synthesis heteroatom and bimetallic clusters. Closed shell electronic requirements for cluster

compounds, introduction to tensor surface harmonic theory of clusters. Metal clusters in catalysis.

Organization of neutral boron hydrides, anionic borane, carboranes and metallocarboranes, outline of the synthesis and properties of C_{60}. Isolobal analogy in organometallic and cluster compounds. *Marks 18*

Recommended Books :

Course 40520 : Elective II
Natural Products Chemistry
Credit – 4

Total Marks -100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time: 3 hours	**3**	**1**	**0**	**4**

Unit I *Marks-20*

Alkaloids – Structure elucidation, reactions and synthesis of the following :

Phenanthrene alkaloid-- Morphine.

Indole alkaloid -- Reserpine, Strychine.

Isoquinoline alkaloid- Emetine

Tropolone alkaloid- Colchicine.

Biogenesis of alkaloids—A general discussion.

Unit II *Marks-18*

Terpenoids – Structure elucidation, synthesis, reactions and stereochemistry of the following :

Farnesol, Zingiberine, Cadinene, Phytol, Abietic acid and Squalene, β-Amyrin.

Biogenetic pathway of mono and sesquiterpenes.

Unit III *Marks-6*

Carotenoids – Occurance, isolation, and structure determination of carotenes, lycopene and xanthophylls.

Unit IV *Marks-8*

General methods of structure determination and synthesis – Anthocyanins, flavones and flavonols.

Unit V *Marks-8*

Porphyrins- Chemistry of heme, oxygen transport of haemoglobin, chemistry of chlorophyll and its role in photosynthesis.

Text books :

1. Organic Chemistry of Natural Products, Vol I and II, Gurdeep Chatwal, Himalaya Publishing House, Bombay.
2. Chemistry of Organic Natural Products, Vol I and II , O.P. Agarwal, Goel Publishing House, Meerut.

Reference books :

1. The Alkaloids Vol I – XVIII – R.H.F. Manske (ed), Academic Press
2. The Alkaloids – K.W. Bentley
3. The Terpenes – Vol. I – IV, Simonsen & Others.
4. The Alkaloids Vol I – XVIII – R.H.F. Manske (ed), Academic Press
5. Chemistry of Natural Products – P.S. Kalsi, Kalyani Publishers, New Delhi
6. Steroids - Fieser and Fieser
7. Synthesis of Natural Products Vol I, IIa, IIb ed, Apsimon
8. The Terpenes – Vol I – IV, Simons & Others.

Course 40530 : Elective II
Advanced Electrochemistry
Credit – 4

Marks -100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time : 3 hours	**3**	**1**	**0**	**4**

Unit I

Thermodynamics of Electrocapillary phenomenon; Surface excess, relevance of outer and surface potential to double layer (DL) studies, surface and inner potential difference. Capacity potential relations in electrode-electrolyte interface, Contact adsorption-its influence on capacity of interface, Capacitance hump. *Marks-15*

Unit II

Eletrode kinetics: Simple Butter–Volmer (BV) equation, exchange currents, over potential, physical meaning of symmetry factor. BV equation for multistep reactions, high and low field approximation. *Marks-15*

Unit III

Electrocatalysis: Definitions, Electrocatalytic potential, effect of electric field on electrocatalysis, *Marks-8*

Unit IV

Cyclic Voltammetry (CV), Randles Sevick equation, properties of potential, properties of current, electrode used in CV. Chronopotentiometry and Chronoamperometry. Impedance Spectroscopy *Marks-12*

Unit V

Electrochemical energy conversion: Direct energy conversion, actual efficiency of an electrochemical energy converter, condition for maximum efficiency, power output of energy convertor. *Marks 10*

Books Recommended:

1. Modern Electrochemistry: Vol II by J. O. M Bockris & A. K. N. Reddy
2. Modern Electrochemistry by Kortum.
3. Inorganic Electrochemistry: Theory, Practice and Applications by Piero Zanello

Course 40610 : Elective III
Bio-inorganic Chemistry
Credit – 4

Total Marks - 100 (End Semester 60+ Internal Assessment 40)	**L**	**T**	**P**	**C**
Time : 3 hours	**3**	**1**	**0**	**4**

Unit I

Role of 3d block elements and non-metals in bio-systems, Essential and trace elements in biological systems, oxygen binding metallo-biomolecules. *Marks 9*

Unit II

Transport and storage of dioxygen, Heme proteins (hemoglobin, myoglobin, cytochrome C) and oxygen uptake, structure and function of Hb, Mb, hemocyanin and hemerythrin, model synthetic complexes of Fe, Co and Cu. *Marks 15*

Unit III

Bioenergetics and ATP cycle, DNA polymerization glucose storage, metal complexes in energy transmission, photosystem I and II in cleavage of water. *Marks 10*

Unit IV

Bioinorganic chemistry of Co, Zn, Cu, Biological fixation of dinitrogen, Cytochrome C oxidase and superoxide dismutase, ceruloplasmin, metal ion transport and storage (transferrin and ferrition), biotransformation of nonmetallic inorganic compounds, Anti-oxidants, metal ions as antioxidants. *Marks 20*

Unit V

Spectral, biochemical and biological methods used in bioinorganic chemistry. *Marks 6*

Recommended Books:

1. Lippard S.J. & Berg J.M, Principles of Bioinorganic Chemistry, Univ. Science Books (1994).
2. Bioinorganic Chemistry by K. Hussain Reddy, New Age International Publishers.
3. Bio-inorganic Chemistry by R.W. Hay, Ellis Horwood Ltd, 1st Published in 1984 and reprinted in 1987 and 1991.
4. Essential of Bio-inorganic chemistry, Dr. N. Gupta & Dr. M. Singh, Pragati Prakashan, 1st Edn. 2008.
5. Bio-inorganic Chemistry; Bertini, Gray, Lippard and Valentine.

Course 40620 : Elective III
Bioorganic Chemistry and Biochemistry
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time : 3 hours	**3**	**1**	**0**	**4**

Unit-I *Marks-15*

Co-enzymes, derived from vitamins, structure and biological functions of Co-enzymine-A, thiamine pyrophosphate, pyridoxal phosphate, lipoic acid and vitamin B_{12}.

Inhibition of enzyme, Concept and identification of active site by the use of inhibitors. Regulatory enzymes.

Enzyme models: Host-Guest chemistry, chiral recognition and catalysis. Cyclodextrin based enzyme models. Crown ethers, cryptates, calixarenes, ionophores, micelles, synthetic enzymes or synzymes.

Unit – II *Marks 15*

Nucleic acids : Genetic code, Replication of DNA, Mechanism of transcription and translation. Biosynthesis of proteins.

Chemical synthesis of DNA, PCR.

Unit-III *Marks 10*

Metabolism of Carbohydrates: Glycolysis and gluconeogenesis, fate of pyruvic acid and Krebs cycle.

Unit IV *Marks 10*

Biochemistry of Lipids: Biological importance of fatty acids and lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, calorific value of foods, biological membranes, properties and functions of lipid bilayers and liposomes. Biosynthesis of fatty acids., triacylglycerols, phospholipids.

Unit V

Steroids and hormones: Occurrence, General methods of isolation, structure determination, synthesis and stereochemistry of cholesterol and bile acid, Synthesis of oestrone, testosterone, progesterone and their therapeutic applications. *Marks-10*

Recommended books:

1. Principles of Biochemistry – A.L. Lehninger, D.L. Nelson and M.N. Cox, CBS Publishers and Distributors
2. Outlines of Biochemistry – E.E. Cohn and Stampf, Wiley Eastern
3. Harper's Biochemistry.
4. Textbook of Biochemistry : U Satyanarayana

Course 40630 : Elective III
Solid State Chemistry
Credit 4

Total Marks 100 (End Semester 60 + Internal Assessment 40)	**L**	**T**	**P**	**C**
Time : 3 hours	**3**	**1**	**0**	**4**

Unit I

Electronic Structure of Solids: Band theory, Formation of Bands, Energy bands in semiconductors, intrinsic and extrinsic type of semiconductors. Formation of p-n junction and its explanation. Forward and reverse Bias. *Marks 15*

Unit II

Solid state transformations: Wagner reaction mechanism of solids, kinetics of solid state reaction, thermal decomposition reaction, Free energy of nucleation, Growth of nuclei.

Marks 15

Unit III

Optical and dielectric properties of solids: Electron emission in Metals, photovoltaic effect, Luminescence, Dielectric properties of solids. *Marks 10*

Unit IV

Super Conductivity: Meisner effect, crytal field effect, B.C.S. Theory, effect of Magnetic field, low temperature superconductivity (LTSC) and high temperature superconductivity (HTSC). Phase-diagram of Y–Ba-Cu–O, Synthesis of Y-$Ba_2Cu_3O_{7-X}$, its crystal structure. Organic superconductors, Fullerene, Applications of superconductors. *Marks 20*

Recommended Books:

1. Principles of the Solid State Chemistry – H.V. Keer, New Age International (P) Ltd.
2. Solid State Chemistry and its applications, by A.R. West, Plenum.
3. Solid State Chemistry by D.K. Chakraborty, New Age International Publishers
4. Solid State Physics by Kittel
5. A text book of Physical Chemistry by H. K. Moudgil

Course 40710: Elective IV
Introduction to Chemistry of Nanomaterials
Credit - 4

Total Marks - 100 (End Semester 60+ Internal Assessment 40)	**L**	**T**	**P**	**C**
Time : 3 hours	**3**	**1**	**0**	**4**

Unit I

Introduction to physics and Chemistry of solids, energy bands: conductor, semiconductor and insulator. Size dependence of properties. Donor, acceptor and deep traps. Exciton.

Methods of measuring properties: crystallography, size of particles, surface structure. Properties of individual nanoparticles: Metal nanoclusters, semiconducting nanoparticles. Synthesis of oxide nanoparticles by Chemical method and by thermolysis. *Marks 20*

Unit II

Carbon nanoclusters and nanotubes, application of CNT in fuel cell, catalysis, computer and as chemical sensors. Polymeric nanofibres, supramolecular structures; nanoparticles organized in/on polymer surfaces. *Marks 20*

Unit III

Magnetic nanostructured particles, electrical and optical properties of nano materials. Quantum wells, wires and dots. Quantum confinement. *Marks 20*

Recommended Book:

Introduction to Nanotechnology *by* C.P. Poole Jr. & F. J. Owens, Wiley India 2006.

Course 40720 : Elective IV
Medicinal Chemistry
Credit - 4

Total Marks - 100 (End Semester 60 + Internal Assessment 40) **L T P C**
Time : 3 hours **3 1 0 4**

Unit – I *Marks-30*

Drugs: Definition of drugs and factors affecting their bioactivity; Definition of chemotherapeutic index and therapeutic index. Quantitative structure activity relationship (QSAR). Concepts of drug receptor, theoretical aspects of drug receptor interaction. Drug introduction, Metabolism, Excretion. Introduction to designing of drugs; Structural modification of drugs. Introduction to combinatorial library of drugs.

Sulphadrugs: Historical significance of sulpha drugs as antibacterial agent, Sulphanilamide and other important sulpha drugs and their mode of action.

Antibiotics : Introduction and classification, Structure action relationship and mode of action of penicillin, semisynthetic penicillins, streptomycin, chloramphenicol and tetracyclins.

Antimalarials: Introduction and classification, human malaria and plasmodia, Chloroquine, mepaquine, trimethopriim and mefloquine – their structure and activity as antimalarials.

Artemisinin and its derivatives, structure-action relationship.

Drugs used for treatment of cancer and tuberculosis and recent developments

Unit – II *Marks-24*

Vitamins: Structure determination, synthesis and physiological activity (role of vitamins as co-enzymes) of the following ; retinal (Vit A_1), 3-dehydroretinol (Vit A_2), thiamine (Vit B_1), Riboflavin (Vitamin B_2) Vitamin B complex, Pantothenic acid, folic acid complex, niacin & dervt.) Biotin (Vit H), Pyridoxine (Vit B_6), Cyanocobalamin (Vit B_{12}) Tocopherols (Vit E) and Phylloquinone (Vit K_1).

Unit – III *Marks-6*

Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE2 and PGE2α

Recommended books:

1. Medicinal Chemistry – A. Kar, Wiley Eastern Ltd., New Age International Ltd., New Delhi
2. Medicinal Chemistry – A. Burger (ed). Interscience, New York
3. An introduction to medicinal chemistry- G.L. Patrick. Oxford University Press.

Course 40730 : Elective IV
Advanced Quantum Chemistry
Credit - 4

Total Marks - 100 (End Semester 60 + Internal Assessment 40) **L T P C**
Time : 3 hours **3 1 0 4**

Unit I

Theoretical and Computational treatment of atoms and molecules, some basic ideas of matrix algebra. Review of the principles of quantum mechanisms: Born-Oppenheimer approximation, Antisymmetry Principle; Hartree product, Slater determinant; Slater-Condon rules; Hartree-Fock equations, Koopmans' and Brillouin's theorems, Roothaan equation's, SCF procedure. *Marks 32*

Unit II

Semi-emperical theories: A review of the Huckel method, Zero differential overlap, Complete Neglect of Differential Overlap and Intermediate Neglect of Differential Overlap theories. *Marks 10*

Unit III

Density functional Theory: Hohenberg-Kohn theorems; *N*- and *v*-representability, Levy constrained search formulation; Kohn-Sham formulation: Introduction of orbitals and KS equations, exchange-correlation functionals; treatment of chemical concepts within the density functional theory. *Marks 18*

Recommended Books :

1. Modern Quantum Theory – N. S. Ostlund and A. Szabo, McGraw Hill.
2. Methods of Molecular Quantum mechanics, R. McWeeney and B. T. Sutcliffe, Academic Press.
3. Density functional theory of atoms and molecules, R. G. Parr and W. Yang, Oxford.
4. Semi-empirical MO Theory – J. Pople and D.L. Beverdge.
5. Quantum Chemistry, I. N. Levine

Course 40810 : Project/ Advanced Inorganic Practical
Credit - 8

Total Marks 200 (End semester 120 + Internal Assessment 80)	**L**	**T**	**P**	**C**
Time : 12 hours	**0**	**0**	**8**	**8**

A. Ligands and Metal Complexes *Marks 80*

1. Synthesis and characterization of some dithiocarbamate ligand and their complexes with transition metals.
2. Synthesis of phosphine chalcogenide ligand ($PPh_3O/PPh_3S/PPh_3Se$) and their complexes.
3. Synthesis of some pyrazolyl borate ligands and their complexes with transition metals.
4. Preparation of some clay based materials. Pillaring of Mont-K-10, Saponite and Vermiculate with transition metal ions and some chalcogenides. Preparation and characterization of polymer clay nano-composites.
5. Preparation of some metal pigments and paints.
6. Synthesis of nano-particles by sol-gel, Co-precipitation, chemical bath deposition and thermolysis method and their characterization.
7. Preparation of metal ceramic particles and their characterization
8. Complete water and soil analysis (including F^- and arsenite)
9. Estimation of Fe, Ca, Mg, K, Na, Zn in certain local fruits/vegetables.

B. Review of literature on topics of recent advances/ selected topic. *Marks 20*

C. Viva-voce *Marks* 20

OR

Research project approved by the Supervisor, preparation of the dissertation and presentation of the results and viva-voce examination by a board of examiners.

Dissertation ***Marks 90***

Viva-Voce ***Marks 30***

Course 40820 :: Project/ Advanced Organic Chemistry Practical
Credit - 8

Total Marks 200 (End Sem 120 + Internal Assessment 80)	**L**	**T**	**P**	**C**
Time : 12 hours	**0**	**0**	**8**	**8**

1. Advanced Practical*, Literature Survey and Viva voce **Marks – 80 + 20 + 20 = 120**

[*Advance practical includes (A) Preparation, purification (by TLC) and spectroscopic identification (UV and IR) of the prepared organic compounds and (B) Estimation]

(A) Preparation **50**

1. Benzilic acid from benzoin via benzyl (Benzilic acid rearrangement)
2. Benzanilide from benzophenone via oxime (Beckman rearrangement)
3. Indigo from anthranilic acid via phenylglycine-o-carboxylic acid and indoxyl
4. Sandmeyer reaction-
   (a) ortho-Chlorotoluene from ortho-toluidine (steam distillation of the product)
   (b) Acridone from anthranilic acid via *o*-chlorobenzoic acid and N-phenylanthranilic acid
5. Sulphanilamide from acetanilide via *p*-acetamidobenzenesulphonylchloride and *p*-acetamidobenzenesulphonamide
6. Pinacolone from benzophenone via pinacol (Pinacol pinacolone rearrangement)

(B) Estimation **30**

i) Estimation of glycine by formalin method

ii) Estimation of halogen by fusion method

iii) Estimation of hydroxyl and amino groups by acetylation method

OR

Research project approved by the Supervisor, preparation of the dissertation and presentation of the results and viva-voce examination by a board of examiners.

Dissertation ***Marks 90***

Viva-Voce. ***Marks 30***

Course 40830 : Advanced Physical Practical
Credit – 8

Total Marks 200 (End Sem 120 + Internal Assessment 80)	**L**	**T**	**P**	**C**
Time : 12 hours	**0**	**0**	**8**	**8**

Adv. Practical + Literature Survey + Viva voce = 80 + 20 + 20

1. Determine the amount of each component of the following ternary mixture by conductometric titration.

   HCl, CH_3COOH, $CuSO_4$

   HCl, NaCl, NH_4Cl

2. Determine the composition of the binary mixture ($K_2Cr_2O_7$ and $KMnO_4$) by spectroscopic method.
3. Determine the ionization constant of acetic acid by conductivity method.
4. To find the stability constant of the co-ordination compound formed between Cu^{2+} and 5-sulphosalicylic acid.
5. Determine the stability constant of $FeSCN^{2+}$ complex at ionic strength of 1. (Least square method)
6. Determine the indicator constant of methyl red.
7. Establish the order reaction for $K_2C_2O_4 + 2HgCl_2 \rightarrow Hg_2Cl_2 + 2KCl + CO_2$ by the method of ratio variation.
8. Investigate the reaction between H_2O_2 and HI (clock reaction). Determine the energy of activation
9. Study the catalytic decomposition of H_2O_2
10. Determine the percentage polymerization of MMA or styrene initiated by AIBN at 60^oC by gravimetric method.
11. To determine the equilibrium constant of the reaction : $KI + I_2 = KI_3$ by distribution method.
12. Compare the clearing power of different samples (at least four) of soaps and detergents by surface tension measurement.
14. Determination of molecular weight of a non-electrolytic substance by Cryoscopic method using benzene as the solvent.
15. Spectroscopic properties of acetone.
16. Determine the partial molar volume of ethanol in dilute aqueous solutions.
17. Determine the formation constant of donor accepter complex formed by pyridine with Iodine by determining the existence of isosbestic point in non-polar solvent.
18. Experiments on Computation Analysis.

OR

Research project approved by the Supervisor, preparation of the dissertation and presentation of the results and viva-voce examination by a board of examiners.

Dissertation	***Marks 90***
Viva-Voce	***Marks 30***

N.B.: New experiments will be introduced from time to time subject to the availability of chemicals and instrument.

BOOKS RECOMMENDED FOR ORGANIC CHEMISTRY :

General Approach :

1. Organic Chemistry, Vols I and II – I. L. Finar, ELBS.
2. Organic Chemistry – R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Prentice Hall India Limited
3. Organic Chemistry – Paula Yurkanis Bruice, Pearson
4. Organic Chemistry – T.W.G. Solomons, John Wiley and Sons, NY
5. Organic Chemistry- Clayden, Greeves, Warren and Wothers, Oxford University Press.
6. Organic Chemistry – Carey and Sundberg
7. Advanced Organic Chemistry Part A and B : Carey and Sundberg
8. Advanced Organic Chemistry : Singh and Yadav

Organic Reaction Mechanism :

1. Advanced Organic Chemistry: Reaction Mechanism and Structure – Jerry March, Wiley Eastern.
2. A Guidebook to Mechanism in Organic Chemistry– Peter Sykes, Longman, New York.
3. Reaction Mechanism in Organic Chemistry – S.M. Mukherji and S.P. Singh, Macmillan

Reagents for Organic Synthesis :

1. Modern Methods of Organic Synthesis – Carruthers and Mendham, Cambridge University Press
2. Organic Synthesis – M.B. Smith, McGraw Hill. (Reference book)
3. Principles of Organic Synthesis – R.O.C. Norman and J M Coxon
4. Organic Synthesis – J. Singh and L.D.S.Yadav, Pragati Prakashan
5. Application of Redox and Reagents in Organic Synthesis- R.K. Kar, New Central Book Agency
6. Fundamentals of Organic Synthesis : The Retrosynthetic Analysis - R.K. Kar, NCBA
7. Synthetic Approaches in Organic Chemistry – R.K. Bansal- Narosa Publishing House, New Delhi
8. Modern Synthetic Reactions – H.O. House, W.A. Benjamin, NY

Stereochemistry :

1. Stereochemistry of Organic Compounds – D. Nasipuri, Wiley Eastern
2. Stereochemistry of Carbon Compounds – Earnest E. Eliel, Tata McGraw Hill
3. Stereochemistry of Carbon Compounds – Subrata Sengupta, New Central Book agency, Kolkata
4. Stereochemistry and Mechanism through Solved Problems- P.S. Kalsi, New Age International Publishers

Heterocyclic Chemistry:

1. Heterocyclic Chemistry : Synthesis, Reactions and Mechanisms – Raj K. Bansal, Wiley Eastern.
2. Heterocyclic Chemistry – T.L. Gilchrist, Longman Scientific and Technical/Pitman Publ. Ltd.
3. The Principles of Heterocyclic Chemistry : Theophil Eicher and Siegfried Hauptnann, RSC
4. Principles of Modern Heterocyclic Chemistry – Leo A. Pacquette, W.A. Benjamin, Inc. New York
5. The Principles of Heterocyclic Chemistry – A.R. Katritzky and J.M. Lagowski, Chapman and Hall Ltd

6. Heterocyclic Chemistry – D.W. Young, Longman Group Lt. London
7. An Introduction to the Chemistry of Heterocyclic Compounds, R.M. Acheson, Wiley International.

Retrosynthetic Analysis:

1. Disconnection Approach in Organic Synthesis – S. Warren, Wiley
2. Designing Organic Synthesis – S. Warren, Wiley, Chichester
3. The Logic of Organic Synthesis – E.J. Corey and Xue Min Chen, Wiley, New York

Organic Photochemistry :

1. Organic Photochemistry – J.M. Coxton and B. Halton, Cambridge University Press.
2. Introductory Photochemistry – A. Cox and T.J. Kemp, McGraw Hill
3. Elements of organic photochemistry – Dwaine O. Cown and Ronald L. Driske, Plenum Press, New York and London
4. Photochemistry and Pericyclic Reactions : J Singh and J Singh, New Age International Publishers
5. Fundamentals of Photochemistry – K.K. Rohatgi-Mukherji, Wiley Eastern

Pericyclic Reactions :

1. Frontier Orbitals and Organic Chemical Reaction – Ian Flaming, John Wiley
2. see Advanced Org Chem Part A and B by Carey and Sundberg

Medicinal Chemistry :

1. Medicinal Chemistry – A. Kar, Wiley Eastern Ltd., New Age International Ltd., New Delhi
2. Medicinal Chemistry – A. Burger (ed). Interscience, New York

Biochemistry :

1. Principles of Biochemistry – A.L. Lehninger, D.L. Nelson and M.N. Cox, CBS Publishers and Distributors
2. Outlines of Biochemistry – E.E. Cohn and Stampf, Wiley Eastern
3. Harper's Biochemistry.
4. Textbook of Biochemistry : U Satyanarayana.

Organic Natural Products Chemistry:

1. Organic Chemistry of Natural Products, Vol I and II, Gurdeep Chatwal, Himalaya Publishing House, Bombay.
2. Chemistry of Organic Natural Products, Vol I and II , O.P. Agarwal, Goel Publishing House, Meerut.

Reference books : (Natural Products)

1. The Alkaloids Vol I – XVIII – R.H.F. Manske (ed), Academic Press
2. The Alkaloids – K.W. Bentley
3. The Terpenes – Vol. I – IV, Simonsen & Others.
4. The Alkaloids Vol I – XVIII – R.H.F. Manske (ed), Academic Press
5. Chemistry of Natural Products – P.S. Kalsi, Kalyani Publishers, New Delhi
6. Steroids - Fieser and Fieser
7. Synthesis of Natural Products Vol I, IIa, IIb ed, Apsimon
8. The Terpenes – Vol I – IV, Simons & Others.