DEPARTMENT OF CHEMISTRY
ASSAM UNIVERSITY: SILCHAR

M.Sc Chemistry Modified Syllabus with effect from 2013-14 Session
Course Structure

Semester	Course Number	Course Name	No of periods per week/ semester	Total Marks			Credit Point
				Internal	*External*	*Total*	
I	CH-101	Inorganic Chemistry – I	4 / 60	25	75	100	5
	CH-102	Organic Chemistry – I	4 / 60	25	75	100	5
	CH-103	Physical Chemistry-I	4 / 60	25	75	100	5
	CH-104	Quantum Chemistry and Chemical Bonding	4 / 60	25	75	100	5
	CH-105	Laboratory Course in Inorganic Chemistry	15 / 225	25	75	100	5
II	CH-201	Inorganic Chemistry – II	4 / 60	25	75	100	5
	CH-202	Organic Chemistry – II	4 / 60	25	75	100	5
	CH-203	Physical Chemistry-II	4 / 60	25	75	100	5
	CH-204	Molecular spectroscopy	4 / 60	25	75	100	5
	CH-205	Laboratory Course in Organic Chemistry	15 / 225	25	75	100	5
III	CH-301	Inorganic Chemistry –III	4 / 60	25	75	100	5
	CH-302	Organic Chemistry – III	4 / 60	25	75	100	5
	CH-303	Physical Chemistry-III	4 / 60	25	75	100	5
	CH-304	Applications of spectroscopic Methods	4 / 60	25	75	100	5
	CH-305	Laboratory Course in Physical Chemistry	15 / 225	25	75	100	5
IV	CH-401	Analytical and Computational Chemistry	4 / 60	25	75	100	5
	CH-402	Chemistry of Advanced Materials	4 / 60	25	75	100	5
	CH-403A/	Inorganic Chemistry-IV	4 / 60	25	75	100	5
	CH-403B/	Organic Chemistry – IV	4 / 60	25	75	100	
	CH-403C/	Physical chemistry-IV	4 / 60	25	75	100	
	CH-404 A/B/C	Project work, Inorganic/ Organic/ Physical	25 / 375	50	150	200	10

Total Marks 2000
Total Credit Point 100

CHEMISTRY – 101: INORGANIC CHEMISTRY - I
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT – I: Symmetry and Structure:
Symmetry elements and symmetry operations, symmetry groups with examples from inorganic compounds, groups of very high symmetry, molecular dissymmetry and optical activity, molecular symmetry for compounds having coordination number 2 to 9, Molecular dissymmetry and polarity, matrix representations of symmetry operators and their products.

UNIT – II: Bonding:
Bond energy and covalent radii. Electro negativity (calculations using Pauling, Mulliken and Allred Rochow methods) and polarity of bonds. Brief review of metallic bonding, band theory, hydrogen bonding, Clathrates and VSEPR model, the use of outer d-orbitals, d□□p□□bonding. Spectroscopic electronegativity, concept of chemical hardness (□). Walsh diagrams (triatomic systems). MO treatment of simple diatomic (homo & hetero) system with special reference toB_2, C_2, N_2, F_2, CO, HCl etc.

UNIT – III: Selected topics on non-transition elements:
Concept of cluster, Wade's rule, Styx number, PSEPT, Synthesis, properties and structures of boranes, carboranes, metallo-carboranes, silicates and S- N and P – N Compounds. Non-Stoichiometric oxides, zeolites and clay. Polymorphism of carbon, phosphorus and sulphur. Peroxo Compounds of B, C and S. Isopoly and Heteropoly anions.

UNIT – IV: Environmental pollution and Bioinorganic chemistry:
Air pollution (CO, CO_2, C budget, C-credit, CO_2 sequestration, SO_x, O_3 and NO_x.
Photochemical Smog (PS) and chemistry of PS formation, Sulphurous Smog.
Water pollution (heavy metals and phosphates), toxicity of Hg, Pb, Cd, Cr and As. Essential and trace elements in biological systems, biochemistry of sodium and potassium, membrane structure, mechanism of ion transport across membranes, biological defense mechanism, ionophores, valinomycin and crown ether complexes of Na and K. Cryptand complexes.

UNIT – V: Kinetics and Mechanism of Inorganic reactions:

Mechanism of ligand replacement reactions, ligand displacement reactions in octahedral and square planar complexes, trans-effect, isomerisation and racemisation in tris-chelate complexes, electrons transfer reactions, Cross-section and Marcus-Hush theory. Stereochemical non-rigidity and fluxionality (concept, examples, techniques of detection)

Suggested Reading:

1. F. Basolo and R. Johnson, Coordination Chemistry, Science Rewiews, Northwood, 1987.
2. R. Debock and H. B. Gray, Chemical structure and bonding, Benjamin/Cummings, Menlo Park, 1980.
3. N. N. Greenwood and A. Earnshaw, Chemistry of the elements, Pergamon, Oxford, 1984.
4. H. G. Heal, The Inorganic Heterocyclic Chemistry of Sulfur, Nitrogen and phosphorus.
5. D. F. Shriver, P.W. Atkins and C.H. Landgord, Inorganic Chemistry, 3rd Edn., Oxford University Press, 1998.
6. J. D. Atwood, Inorganic and Organometallic reaction mechanisms, 2nd Edn. 1997, VCH Publishers, New York.
7. S. E. Manahan, Environmental Chemistry, Lewis Publishers.
8. C. Baird, W. H. Freeman, Environmental Chemistry.
9. G. L. Miessler and D. A. Tarr, inorganic Chemistry, Pearson. 2009.
10. J. D. Lee, Concise Inorganic Chemistry, Chapman & Hall Ltd., 1991
11. G. Wulfsberg, Inorganic Chemistry, Viva Books Pvt. Ltd. 2002.
12. A. K. Das, Fundamental concepts of inorganic chemistry, Vol III, Second Edn. CBS, 2010.
13. G. N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, U. N. Dhar & Sons Pvt. Ltd.,1993
14. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, Addison – Wsley Publishing Company, 1993

Additional Reading:

1. W. L. Jolly, Inorganic Chemistry, 1976, McGraw Hill, New York.
2. J. E. Fergusson, Inorganic Chemistry and the Earth: Chemical Resources, Use and Environmental Impact, Vol. 6, Pergamon Press, Oxford, 1982.
3. S. F. A. Kettle, Symmetry and Structure, Wiley, New York, 1985.
4. D. C. Harris and M.D. Bertolucci, Symmetry and Spectroscopy, Oxford University Press, 1978.

CHEMISTRY – 102 : ORGANIC CHEMISTRY – I
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT – I: Nature of bonding in organic molecules:
Delocalised chemical bonding-conjugation, resonance, hyperconjugation, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds. Huckel's rule, energy level of -molecular orbitals, annulenes, antiaromaticity, homo-aromaticity. Crown ether complexes and cryptands, cyclodextrins, catenanes and rotaxanes. Nanotubes and nano rods. Study of Fullrenes. Hydrogen bonds, nonbonding intermolecular forces. Effect of structure on reactivity – resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants.

UNIT : II : Basic concepts of stereochemistry :
Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Chirality, molecules with more than one chiral centres, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Methods of asymmetric synthesis including chiral pool, chiral auxiliary, chiral reagents; enantio and diastereo selective and specific synthesis. Inclusive of substrate control and reagent control strategies eg, Sharpless epoxidation and di-hydroxylations with AD-mix-□ and □.

UNIT : III Substitution reactions (aliphatic and aromatic):
Review of SN2, SN1, SNi along with mixed SN^1 and SN^2 and SET mechanisms. Carbocation: Classical and non-classical: Generation, stability and classification and as reaction intermediates. The neighbouring group mechanism, neighbouring group participation by π and σ bonds (anchimeric assistance). Nucleophilic substitution at an allylic, aliphatic trigonal and at vinylic carbon. Leaving group and ambident nucleophile, regioselectivity. Diazonium coupling, Ipso substitution, Vilsmeir Haak reaction, Gattermann-Koch reaction. The Sommelet-Hauser, and Smiles rearrangements.

UNIT : IV CARBONYL AND RELATED GROUPS
Nucleophilic addition, hetero atoms (N, O) Hydride donors as nucleophiles, carbanion additions, addition elimination and stereo selective aldol type of condensations. Enolates, emines and enamines: their roles in chemoselective and regioselective C-C bond formations. Alkylation of enolates, emines and enamines and their stereochemical outcomes. Vinylogous or conjugate additions. Substitution by hydrides and acylation of carbon, carbonyl cyclization reactions and cleavage of carbonyl compounds..

UNIT: V ADDITION AND ELIMINATION REACTIONS:
Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds- stereochemical aspects including Cram's rule. Wittig, modified Wittig reaction.
Introduction to Elimination reactions: formation of alkenes by eliminations with proton loss and by other elimination reactions including 6-membered cyclic substrate. Formation of other double bonds (C = N, C = O) and triple bonds by elimination reactions. Stereochemistry of elimination reactions. Pyrolytic syn-Elimination reactions of esters, xanthates and sulfoxides.

ESSENTIAL READINGS :

1. L. N. Ferguson – The modern structural theory of organic chemistry, Prentice Hall of India (1973).
2. L. Pauling – Nature of the chemical bond, Cornell University Press (1960).
3. T.W.G. Solomons – Organic chemistry, John Wiley (1992).
4. D. Nasipuri – Stereochemistry of Organic compounds, Wiley Eastern (1994).
5. Seyhan Ege – Organic chemistry (Structure and reactivity, 3rd Edn., 1998), AITBS Publishers, Delhi.
6. F. A. Carey and R. J. Sandberg, Plenum.
7. P. Y. Bruice, Organic Chemistry, Pearson Education, inc 2002.

ADDITIONAL READINGS:

1. J.C. Stowell, Intermediate organic chemistry John Wiley.
2. T.W.G. Solomons, Organic chemistry and study guide to accompany organic chemistry, 5th Edn., John Wiley.
3. J.B. Hendrickson, D.J. Cram and G. Hammond – Organic chemistry, McGraw Hill (1970).
4. E.L. Eliel – Stereochemistry of carbon compounds, McGraw Hill, Book Company Inc. (1960).
5. J. March – Advance organic chemistry; Reactions mechanism and structures, 4th Edn. , Wiley Eastern.
6. J. Clayden, N. Greeve, S. Warren and P. Wother – Organic Chemistry, OUP, New Delhi-200001.
7. M. B. Smith – Organic Synthesis, McGraw Hill 1994.

CHEMISTRY – 103 : PHYSICAL CHEMISTRY – I
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT : I Equilibrium Thermodynamics – I :

Brief review of the concepts of laws of thermodynamics: state and path functions, exact and inexact differentials, zeroth and first law, isothermal and adiabatic processes.
Second law: Thermodynamic view of the entropy, Carnot Cycle, Clausius inequality, Helmholtz and Gibbs free energies, Maxwell's relations.
Third law: Nernst heat theorem, Residual entropies.

UNIT : II Equilibrium Thermodynamics – II :

Thermodynamics of ideal and real gases and gas mixtures, mixing of gases, fugacities of gases and their determination, chemical potentials of liquids and liquid mixtures.
Thermodynamics of ideal and non-ideal binary solutions, excess functions for non-ideal solutions, regular solutions. Thermodynamic criteria for chemical equilibria, equilibrium constant of chemical reactions, dependence of equilibrium constant on temperature and pressure.
Phase equilibrium, derivation of the Gibbs phase rule. Partial molar properties, the Gibbs – Duhem equation, the chemical potential and its significance.

UNIT: III Non-Equilibrium Thermodynamics :

Thermodynamic functions for non-equilibrium states, entropy production and entropy flow, transformations of the generalized fluxes and forces, phenomenological equations, Microscopic reversibility and Onsager's reciprocity relations, electrokinetics phenomena, diffusion, electric conduction, the stationary non-equilibrium states.

UNIT : IV Chemical Kinetics – I :

Arrhenius equation, statistical derivation of activated complex theory. Comparison of absolute reaction rates with those of collision theory. Thermodynamic formulation of reaction rates. Reactions in solution. Comparison of gas and liquid phase reactions. Primary and secondary salt effects (kinetic salt effect). Effects of solvent (concept only) and ionic strength on rate constants.

UNIT : V Chemical Kinetics – II :

Complex reactions, Mechanisms of chain, photochemical and oscillatory reactions, homogeneous catalysis, Kinetics of enzyme reactions, study of fast reactions by flow methods, relaxation methods, flash photolysis and the nuclear magnetic resonance method.

ESSENTIAL READING:

1. P. W. Atkins – Physical Chemistry, 7th Edn. Oxford (2000).
2. I. N. Levine, Physical Chemistry, 4th Edn., McGraw Hill, New Delhi, (1995).
3. G. K. Vemulapally, Physical Chemistry, Prentice Hall, India, 1997.
4. I. Prigogine – Introduction to Thermodynamics of Irreversible processes, Interscience Publ. (1961)
5. K. J. Laidler, Chemical Kinetics, Harper & Row.
6. RP Rastogi and Mishra, Chemical thermodynamics, PHI New Delhi

ADDITIONAL READING:

7. V. Fried, U. Blukis and H. F. Hameka – Physical Chemistry Macmillan (1975).
8. K. J. Laidler & J. H. Meiser, Physical Chemistry, Houghton Mifflin Company, Bonton, 1998.
9. I. N. Levine, Physical Chemistry, McGraw Hill, New York, 1988.
10. Y. A. Gersimov, Physical Chemistry, Mir Publishers, Moscow, 1985.
11. J. Rajaram & J. Kuriakose, Kinetics and Mechanism of Chemical Transformations, McMillan India, 1993.

CHEMISTRY – 104 : QUANTUM CHEMISTRY AND CHEMICAL BONDING
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT - I : Schordinger Wave Equation and its Applications :

Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems.
Schordinger equation - particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator, rigid rotator.

UNIT – II: Angular Momentum, Solution of Schordinger equation for Hydrogen Atom and Approximate Methods:

Angular momentum – Commutation relations, Step-up and Step-down operators for angular momentum.
Hydrogen atom-wave functions of hydrogen atoms, space quantization, Zeeman effect spin-orbit coupling.
Approximate methods: Perturbation theory for non-degenerate states and its applications, variation theorem and its application, Qualitative treatment of Hartree-Fock model in atoms, Roothaan's solution.

UNIT – III: Molecular Orbital and Valance Bond Theory of Diatomic Molecule:

Born-Oppenheimer approximation, Hydrogen molecules ion, LCAO-MO And VB treatment of the Hydrogen molecules, Electron density, forces and their role in chemical binding, LCAO-MO treatment of Heteroneuclear diatomic molecules non-crossing rule and correlation diagram (both homonuclear and heteronuclear diatomics) types of molecular orbitals, isoelectronic principle.
Comparison of Molecular Orbital and Valence Bond Methods Charge densities and polarity, equivalence of the M.O. and V. B. Methods, configuration interactions.

UNIT – IV: Chemical Bonding – I :

Localised bonds in poly atomic molecules – bond properties non-localised orbitals (water molecule as an example), equivalence of pairing approximation, principal types s-p hybridization, factors determining molecular shapes, atomic radii, bond length and bond energies. Simple Huckel Theory, effective one electron Hamiltonian for pi systems, Pi electron approximation, simple Huckel treatment of ethylene, allyl and butadiene systems, charge densities and bond orders, simple formula and diagrammatic methods for calculating the energies and cyclic polyenes.

UNIT – V: Chemical Bonding – II :

Huckel rule for armaticity and anti aromaticity, limitations of simple Huckel model, Wave functions as bases for irreducible representations, projection operators, symmetry adapted linear combinations (SALC), symmetry factoring of secular equations, a few examples of conjugated molecules, HMO methods for hetero atomic compounds, Vanishing of integrals, alternant and odd alternant hydrocarbons, charge densities (unpaired spin densities).

ESSENTIAL READING:

1. A. K. Chandra – Introductory Quantum Chemistry, Tata McGraw Hill (1991).
2. D.A. McQuarrie – Quantum Chemistry, Oxford University Press (1983).
3. P.W. Atkins et al Molecular Quantum Mechanics, OUP, 1998.
4. R. McWeeny – Coulson's Valence, ELBS (1979). Oxford University Press, 1997.
5. R. K. Prasad, Quantum Chemistry, New Age International, New Delhi, 1997.

SUGGESTED READING:

6. Strauss Quantum Chemistry Mechanics, Prentice Hall, 1972.
7. L. Pauling & Wilson, Introduction to QM McGraw Hill , New York, 1935.
8. Eyring, Walter & Kimball, Quantum Chemistry, John Wiley & Sons INC, 1944.
9. J.Calais Quantum Chemistry Workbook, New York, Wiley, 1994.
10. F. A. Cotton – Chemical Applications of Group Theory, W. E. 1992.

CHEMISTRY – 105 : LABORATORY COURSE IN INORGANIC CHEMISTRY
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

1. **SEMIMICRO QUALITATIVE ANALYSIS ;**
   Complete systematic analysis of Inorganic mixtures containing six ions including two of the following elements: W, Mo, Au, Pt, Pd, Se, Te, V, Ti, Zr, U, Th and Ce and the interfering anion (arsenates/phosphate/borate/fluoride).

2. **Quantitative estimation** (involving volumetric-redox and complexometry, gravivimatric and Spectrophotometric methods) of constituents in two and three component mixtures and alloys.

3. **Preparation of the following compounds** : related complementary work and physical studies (at least 8 preparations are to be completed by turn)

a) Reinecke Salt.
b) Trist (Oxalato) manganese (III).
c) Tetrapyridinesilver (II) Peroxodisulphate.
d) Tris (acetylacetonato iron (III).
e) Tris (acetylacetonato (III).
f) Bis (n, N-diethyldithiogarbamato) nitrosyliron (II).
g) Optical isomers of tris (ethylenedimane) cobalt (III) chloride
h) Linkage isomers of dithiocyanato bis (triphenylarsine) Palladium (II) or Nitro and Nitritopentamminecobalt (III) chloride.
i) Ferrocene or dibenzene chromium.
j) Hydrodochlorocarbonyl tris (triphenylphosphine) ruthenium (II).
k) Tetrapyridinesilver (II) nitrate (byelectrochemical methods).
l) Beryllium acetate, $Be_4 O (OCOCH_3)_6$
m) $(PMCl_2)_3$
n) Tris (2, 2-bipridine) ruthenium (II) perchlorate.
o) Dipyridineiodine (I) Nitrate.

4. Physical studies includes magnetic susceptibility conductance measurements, infrared, UV-Visible Spectroscopy and cyclic voltammetry.

ESSENTIAL READINGS ;

1. A.I. Vogel, Macro and Semicro qualitative Inorganic Analysis, Orient Longman, 1969.
2. J. Basset, R.C. Denney, G.H. Jeffery and J. Memdham, Vogel's Text Book of quantitative Inorganic Analysis, ELBS, 4th Edn., 1978.
3. H. H. Willard, L. L. Merrit and J.A. Dean, Instrumental methods of analysis, East-West Press, 4th Edn, 1974.
4. G.W. Parshall (Ed. In chief), Inorganic Synthesis, Vol 15, McGraw Hill, P. 48, 1974.
5. D. D. Sood, S. B. Mohaharand, A. V. R. Reddy, Experiments in Radiochemistry Theory and Practice, IANCAS Publications, 1994.
6. W.L. Jolly : Synthesis and characterization of inorganic compounds Prentice Hall Inc

CHEMISTRY – 201: INORGANIC CHEMISTRY – II
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

Unit – I: **Magnetic properties of transition metal complexes** :
Brief review of different types of magnetic behaviors, spin-orbit coupling, quenching of orbital angular moments, temperature independence paramagnetism. Term symbols for metal ions, crystal field theory and its application to explain magnetic properties of coordination compounds, spin crossover. Magnetic interactions in poly nuclear systems, types of exchange interactions, canting, spin frustration.

Unit – II: **Electronic structure of transition metal complexes** :
Electronic absorption spectra of octahedral and tetrahedral complexes, orgel diagrams, selection rules, band intensities and band widths, spectra of high spin octahedral and tetrahedral complexes for various d^n configurations, spectrochemical series. Adjusted crystal field theory, Nephelauxetic series, Molecular orbital theory of complexes (qualitative principles involved in complexes with no π- bonding and with π-bonding), Charge-transfer transitions of inorganic coordination compounds (different type).

Unit – III : **Aspects of transition elements lanthanides and actinides** :
Elements of first transition series and their comparison with the second and third series, general periodic trends, chemistry to the various oxidation states of first row transition metals and their comparison based on electronic configuration. The splitting of f-orbitals in octahedral field, Lanthanide contraction, Lanthanide shift reagent , oxidation states complexes, magnetic and optical properties of lanthanides and actinides.

Unit – IV : **Transition metal π-acid complexes** :
Structure, bonding, synthesis and reactivity of complexes with CO, OS_1, N_2, NO group V donor ligands and extended π-system ligands (phen, bipy), metal carbonyl hydrides and metal carbonyl clusters : LNCC and HNCC Wale's rule and the Capping rule.

Unit – V : **Aspects of Bioinorganic chemistry** :
Iron-sulphur proteins: Rubredoxin and ferredoxins, metalloporphyrins, Heme Proteins : Hemoglobin, Myoglopin and Cytochrome C, Non-heme proteins : Hemerythrin and Ferritin, Hemocyanin, Nitrogen fixation and introgenases, photosynthesis PSI and PSII.

Essential Readings :

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Eastern Ltd., 3rd. Edn., 1972, 6th edn 1999.
2. J. E. Huheey, E. A. Keiter and R. J. Keiter, Principles of Structure and reactivity, Harper Collins College Publishers, 4th Edn., 1993.
3. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, New York, 1968.
4. M. N. Hughes, The Inorganic Chemistry of Biological Processes, Wiley, 1981.
5. E. I. Ochiai, Bioinorganic Chemistry – An Introduction, Allyn and Bacon, Inc., 1977.
6. Asim K. Das, Bioinorganic Chemistry, Books & Allied (P) Ltd., Kolkata
7. P K Bhattacharya, Metal ions in Biochemistry, Narosa, New Delhi
8. N. Gupta, and Monal Singh, Essential of Bio-inorganic chemistry, Pragati Prakashan.

Additional Readings:

1. B.F.G.Johnson Transition metal clusters, John Wiley 1980
2. T. Moeller, Inorganic Chemistry – A modern Approach, John Wiley, 1982.
3. BN Figgs Introduction to ligand field theory Wiley Eastern Ltd, 1976
4. ABP Lever Inorganic electronic spectroscopy
5. RL Carlin Magnetochemistry Springer Verlag New York 1986
6. O. Kahn, Molecular Magnetism, VCH, New York, 1993

R. L. Datta and A. Syamal, Elements of Magnetochemistry, 2nd Edn, East-west press, New Delhi, 1993.

CHEMISTRY – 202: ORGANIC CHEMISTRY
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT I: Reductive reaction:
A) Introduction to catalytic hydrogenation, reduction of functional groups, Raney Nickel desulphurization. Heterogeneous catalytic hydrogenation (Wilkinson's catalyst) **B) Dissolving metal reduction**, acyloin condensation. **C) Reduction of carbonyl compounds with metal hydrides**, stereochemistry and mechanism of reduction reaction of other functional groups by metal hydrides, Merwein Pondorf Verley reduction, Hydroboration and related reactions including alkyl borane. Tributyl tin hydride (including its coupling reactions). D) Reduction with Hydrazine and its derivatives: The Wolf-Kishner reduction and related reduction of tosylhydrazone, reduction with diimide, reduction employing hydrazine and hydrogenation catalysts.

Unit II: Oxidation Reactions
A) Oxidation with Chromium and Manganese compounds: Oxidation of alcohol, aldehydes, carbon cabon double bonds and carbon–hydrogen bonds in organic molecules, pyridinium chloro chromates (PCC) oxidations. **B) Oxidation with peracids and other peroxides**: Oxidation of carbon-carbon double bonds Sharpless asymmetric oxidation, oxidation of carbonyl compounds, Baeyer–Villigar oxidation. **C) Other methods of oxidation**: Prevost and Woodward, Swern, Moffatt, DMSO-SO_3 complex, Dess-Martin periodinane, iodobenzene diacetate and periodates, thallium nitrate, Ruthenium tetraoxide.

UNIT – III: A) Carbocations: Rearrangements involving carbocations, (Meerwein, Pinacol-pinacolone, Tiffeneau-Demjanov, Dienone phenol, Fries) **B) Carbenes**: Singlet and triplet species- their characteristics, generation, and reactions involving cycloadditions, C-H insertion, nucleophilic reactions and rearrangements (including Wolf, Diazo-ketone reactions including Arndt-Eistert), their stereochemical outcomes of reactions. **C) Nitrenes**: generation structure reactions, and rearrangements (aziridine formation, C-H insertion, Hoffman Curtius and Schmidt) D) **Benzyne**: generation structure, reactions. **E) Phosphorous, nitrogen and sulphur ylides**: methods of generation and reactivity and applications.

Unit IV: A) Free Radicals: Reactions, coupling, addition and substitution, fragmentation, rearrangements inter and intra molecular C-C bond formation.
B) Photochemistry: photosensitization, energy transfer reactions photo-dissociation, gas phase photolysis, photochemistry of alkynes, intramolecular reactions of the olefinic bonds, geometrical isomerism, rearragements of 1,4 (di-pi-methane) and 1,5 dienes, photochemistry of carbonyl compounds including Patterno Buchi (oxitane formation) , Norrish Types I and II (intramolecular reactions of carbonyl compounds) intermolecular cycloaddition reactions and photochemistry of aromatic compounds, photooxygenation and reduction and rearrangements, (Barton, photo Fries), photochemistry of vision and vitamin D.

Unit V:PERICYCLIC REACTIONS :
Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motions, 4n, 4n + 2 and allyl systems. Nazarov Cyclization, cycloadditions – antarafacial and suprafacial additions, 4n and 4n + 2 systems, 2 + 2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements – suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements. Claisen, Cope, aza and oxy-Cope rearrangements. Ene reaction.

Suggested reading :

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, John Wiley
2. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
3. Modern Organic reactions, H. O. House, Benjamin.
4. Principle of organic synthesis, R.O.C. Norman and J.M.Coxon, Blackie Academic & Professional.
5. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
6. P. Y. Bruice, Organic Chemistry, Pearson Education, inc 2002.

Additional reading:

1. Organic Chemistry Michael B. Smith 2000
2. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
3. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
4. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.
5. Principles of organic synthesis R.O. C. Norman and Coxon ELBS
6. Advanced Organic chemistry, F.A. Carry and R.J. Sundberg, Plenum.
7. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.

CHEMISTRY – 203 : MOLECULAR SPECTROSCOPY
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

Unit – I : Basic principles :

Interaction of electromagnetic radiation with matter, time-dependent perturbation theory, harmonic perturbation and transition probabilities, Einstein transition probabilities, selection rules.

Electronic spectra : Introduction to Electronic spectra , Born-Oppenheimer approximation, vibrational course structure: Franck – Condon principle, change of shape on excitation, Jablonski diagram: fluorescence and phosphorescence

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Unit – II : Infra-red spectra :

Vibrational spectra : Harmonic and anharmonic oscillators, fundamental frequencies, overtones, Morse potential, hot bands, vibration-rotational spectra of HCl, PQR branches, vibrational theories of polyatomic molecules, characteristic stretching frequencies of common functional groups and their dependence on chemical environment.

Unit – III : Raman spectra and microwave spectra

Raman Spectra : Molecular polarizability – Raman Effect, pure rotational Raman spectra of linear molecules, vibrational Raman spectra – Raman activity of vibrational, rule of mutual exclusion.

Microwave spectra: rigid and non-rigid rotator models, rotational energies of diatomic molecules: moment of inertia and bond length, centrifugal distortion, effect of isotopic substitution

Unit – IV : Magnetic Resonance :

Spin angular momentum and magnetic moments of electron and nuclei, interaction of magnetic moments with external magnetic field and the relevant Zeeman levels, requirements for inducing transitions between Zeeman levels and detection of magnetic resonance adborption selection rules, field frequency values for ESR and NMR of 1H and 13C, Zeeman interaction for nuclei including the screening by electronic environment, chemical shifts and origin of chemical shifts, chemical shifts in electron system and neighbouring group anisotropy effects with respect to proton chemical shifts, chemical shifts ranges for different nuclei, spectral features due to spin-spin interaction in NMR classification of NMR spectra, desirability of working at higher magnetic fields from the point of view of J\S ratio (measured in Hz and not in ppm).

ESR Spectra : Introduction, the position of ESR adsorption, the g factor fine structure of ESR absorption, hyperfine structure.

Unit – V : Magnetic Resonance :

System of one electron and one nucleus : Zeroth order Hamiltonian, isotropic hyperfine interaction and dipolar interaction between the electron and nucleus, effects of these interaction between electron and nucleus, effects of these interaction as perturbations in the total Hamiltonian for the system of one electron and one nucleus in the presence of an external magnetic field. Basic function for single spin system and product functions for two spin systems, calculation of zero order energies, spin angular momentum operators and identification of pure ESR transitions and NMR transitions in the energy level diagram. Treatment of isotropic (;hyperfine interaction, calculation of first-order and second-order energies and the relevant energy level diagrams, identification of allowed and forbidden transitions. Dipolar coupling tensor for the interaction of two nuclear spins, expression for Hamiltonian in polar coordinates and with raising and lowering spin operators, calculation of coupling constant in dipolar coupled NMR spectra and application to structural studies, first moment and second moment of NMR lines and application to structural studies. Mechanism of hyperfine coupling, McConnell's relation, hyperfine coupling to 13C and 14N nuclei, g-tensor and hyperfine tensor of inorganic radicals, ESR spectra of transition metal ions.

Essential reading:

1. Modern Spectroscopy, J. M. Hollas, John Wiley.
2. Physical Chemistry A molecular approach D.A. McQuarrie, Viva publishers NewDelhi 1998
3. Introduction to Magnetic Resonance, A. Carrington and A.D. Maclachalan, Harper & Raw.
4. Modern Spectroscopy JN Hollas John Wiley, 1990

Suggested reading:

1. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F. L. Ho. Wiley Interscience.
2. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
3. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
4. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.

CHEMISTRY – 204 : PHYSICAL CHEMISTRY – II
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

Unit – I : Equilibrium Electrochemistry :

Activity coefficients of electrolytes, mean activity coefficient, theoretical calculation of activity coefficients Debye-Huckel theory, Debye Huckel limiting law, Ions and Electrodes, electrochemical potential, interfacial potential difference, electric potential at interfaces. Electrochemical cells: EMF and electrode potentials, concentration – dependence of EMF, membrane potentials, thermodynamic data from cell EMF. Ion solvent interactions : The Born model, entropy and enthalpy of ion-solvent interactions.

Unit – II : Dynamic Electrochemistry :

Processes at electrodes: double layer at interface, different models of double layers, rate of charge transfer, over potential, aspects of current-voltage relations, ButlerVolmer equation, Tafel plot, i-v curves, deviations from equilibrium.
Electrochemical processes: Dissolution and deposition at electrodes – currents affecting potential of a cell, power generation and storage process fuel cells – power shortage.
Corrosion: Thermodynamics of corrosion, kinetics of corrosion, and inhibition of corrosion.

Unit – III : Solid State :

Solid state reactions : General principles, experimental procedures co-precipitation, precursor to solid state reaction kinetics of solid state reactions.

Crystal defects: Perfect and imperfect crystals, types of defects (Schottkey and Frenkel defects) colour centres, vacancies and interstitials.

Solid solutions : Requirements for solid solutions, substitutional solid solutions, interstitial solid solutions, Mechanism of solid solutions, creating vacancies of different types.

Electronic properties and band theory: Metals, insulators and semiconductors electrical properties of solids, electronic structure of solids, band theory Brillion Zone superconductors.

Unit – IV: Surface Phenomena :

Surface tension and surface free energy, interfacial tension, adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm: estimation of surface area of solids.
Photoelectron Spectroscopy: Basic principles of UV-photoelectron, X-ray photoelectron spectroscopy and Auger spectroscopy, their applications for chemical analysis of solid surfaces.

Unit – V : Micelles :

Surface active agents, classifications of surface active agents, micellization, hydrophobic interactions, critical micelle concentration (CMC), factors affecting the CMC of surfactants, thermodynamics of micelle formation- phase separation and mass action models, kinetics of micelle formation, solubilization, reverse micelles, micro-emulsions, Kraft phenomenon.

Essential reading:

1. Physical chemistry, P.W. Atkins, OUP, 7th edition 2000
2. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
3. Solid state Chemistry AR West, John Wiley NY 1987
4. Micelles, Theoretical and applied Aspects, Y. Moroi, Plenum, 1992.
5. A whiff on photoelectron spectroscopy, P.K. Ghosh

Suggested reading:

1. Physical chemistry, G.K.Vemulapalli, PHI 1998
2. Principles and applications of electrochemistry DR Crow, 3rd edn Chapman and Hall 1988
3. Experimental approach to electrochemistry NJ Selley, Edward Arnold London 1977

CHEMISTRY – 205: LABORATORY COURSE IN ORGANIC CHEMISTRY
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10
(at least five of the following)

1**. Qualitative Analysis**:
Separation, purification and identification of compounds of binary mixture (one liquid and one solid, two solids) using TLC and column chromatography, chemical tests (Semi micro/Spot test/Capillary method), UV and IR Spectra to be used for functional group identification.
2. **Chromatography**: TLC and column chromatography (CC). Separation and identification of mixture of two or three compounds by chromatography, determination of RF values.

3. **Organic Synthesis: (Any four)**
Acetylation : Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography. **Oxidation**: Adipic acid by chromic acid oxidation of cyclohexanol.
Grignard reaction: Synthesis of triphenylmethanol from benzoic acid. **Aldol condensation**: Dibenzal acetone from benzaldehyde. **Sandmeyer reaction :** p-Chlorotoluene from p-toluidine. Acetoacetic ester condensation synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation. **Cannizzaro reaction**: 4-Chlorobenzaldehyde as substrate. **Friedel Crafts Reaction :** β-Benzoyl propionic acid from succinic anhydride and benzene. **Aromatic electrophilic substitutions** : Synthesis of p-nitroaniline and p-bromoaniline. **Benzilic acid rearrangement**: Benzilic acid from benzoin, Benzoin—Benzil—Benzilic acid . **Synthesis of heterocyclic compounds - Skraup synthesis**: Preparation of quinoline from aniline, **Fisher – Indole synthesis**: Preparation of 2-phenylindole from phenylhydrazine. **Enzymatic Synthesis: Enzymatic reduction:** reduction of ethyl acetoacetate using Bakers' yeast to yield enantiomeric excess of S(+) ethyl-3-hydroxybutanoate and determine its optical purity. Biosynthesis of ethanol from sucrose. Synthesis using microwaves. Alkylation of diethyl malonate with benzyl chloride. Synthesis using phase transfer catalyst. Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide.

4.Extraction of Organic compounds from Natural sources : (Any two)
Isolation of caffeine from tea leaves. Isolation of nicotine dipicrate from tobacco. Isolation of cinchonine from cinchona bark. Isolation of piperine from black pepper. Isolation of lycopene from tomatoes. Isolation of β-carotene from carrots. Isolation of oleic acid from olive oil involving the preparation of complex with urea and separation of linoleic acid). Isolation of eugenol from cloves. Isolation of (+) limonine from citrus rinds
5. **Quantitative Analysis: (any two)**
Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines/phenols using bromate bromide solution or acetylation method. Determination of lodine and Saponification values of an oil sample. Determination of DO, COD and BOD of water sample.
6. **Estimations:** Ascorbic acid, Aspirin, Caffeine.
7. **Use of Computer in organic chemistry**: Simple operations like Drawing of structures, Optimization etc.

ESSENTIAL READINGS :

1. F. Brians, J. H. Antony, P. W. G. Smith and R. T. Austin, Vogel's text book of practical organic chemistry, ELBS, 5th Edn. 1991.
2. R. K. Bansal, Laboratory manual of organic chemistry, 3rd Edn. Wiley Eastern Limited, 1994.
3. D. H. Williams and Ian Fleming, Spectroscopic methods in organic chemistry, TMH Edition, 1988.
4. A. Buzarbarua, A Text Book of Practical Plant Chemistry, S. Chand and Company Ltd., 2000.
5. S. Sadasivam and A. Manikam, Biochemical Methods, Wiley Eastern, 1992.
6. D. L. Pavia, G. M. Lampman and G. S. Kriz, Introduction to Spectroscopy, 3rd Edn. Harcourt College Publishers, 2007.

ADDITIONAL READINGS:

1. A.Y. Sathi, A first courses in food analysis: New Age International (P) Ltd. Publishers, New Delhi, 1999.
2. M. R. Silverstein, C. G. Bassler, C. Horril, Spectroscopic Identification of Organic compounds, John Wiley and Sons, 1991.
3. P. S. Kalsi, Spectroscopy of Organic Compounds, New Age International Publishers Ltd., 1995.
4. I. L. Finar, Organic Chemistry Vol. 2, ELBS with Longman, 1975.
5. H. T. Clarke, A Hand book of Organic analysis Edward Arnold Ltd 1960.

CHEMISTRY – 301: INORGANIC CHEMISTRY – III
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT – I: Organometallic Chemistry:
Synthesis, structure, bonding and reactivity of transition metal complexes with Alkyls, Aryls, Alkenyls, Acyls, Alkynyls. Reactions of (σ-organyls): Homolytic cleavage, Reductive elimination, Electrophilic cleavage, β-metal hydrogen Elimination, α-elimination.
Metal-metal multiple bonds: major structural types, quadrupole bonds, relations of clusters to multiple bonds, one-dimensional solids.

UNIT – II: **Homogeneous catalysis:**
Coordinative unsaturation, oxidative addition reactions, insertion reactions, reaction of coordinated ligand and activation of small molecules by complexation, cayalytic reactions of alkenes (isomerization, hydrogenation, hydroformylation, hydrosilylation and polymerization).

UNIT – III: **Symmetry group theory and its applications:**
Matrix representation of groups, reducible and irreducible representation, the Great Orthogonality Theorem, character tables. Application of group theory: Transformation properties of atomic orbitals, hybridization scheme of σ and π - bonding, hybrid orbitals as LCAO. M.O. theory for AB_n – type molecules e.g. BF relationship of MO and the hybridization treatment, determinations of symmetry types of the normal modes for AB types of system, selection rules, for fundamental vibrational transitions (Infrared and Raman).

UNIT- IV: Nuclear and Radiochemistry:
Radiation detection and measurement, ionization chamber, Geiger-Muller counter, proportional counter, scintillation counter, solid state active and passive detectors, detection of neutrons. Nuclear reactions: Energetics, Q-value, cross-sections types of nuclear reactions, nuclear fission and fusion chain reactions.

UNIT- V: Supramolecular chemistry:
Concepts of language a) **Molecular recognition**: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition.
b) Supramolecular reactivity and catalysis. c)Transport processes and carrier design.
d) Supramolecular photochemistry. e) Supramolecular devices: Supramolecular electronic, ionic and switching devices. f) Some examples of self-assembly in supramolecular chemistry.

Suggested Reading:

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Eastern, 6th Edn. 1999.
2. F. A. Cotton, Chemical Application of Group Theory, Wiley Eastern, 2nd Edn. 1972.
3. G. Friedlander, J. W. Kenendy and J. M. Miller, Nuclear and Radiochemistry, Wiley Int. 2nd Edn. 1964.
4. H. J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1988.
5. R. H. Crabtree, The organometallic chemistry of transition metals, John Wiley, 2nd Edn., 1994.
6. J. M. lehn, Supramolecular Chemistry- Concepts and Perspectives, VCH, Winheim, 1995
7. P. D. Beer, P. A. Gale and D K. Smith, Supramolecular Chemistry, Oxford Scince Publications, 1999.
8. K. Ariga and T. Kunitake, Supramolcular Chemistry,-Fundamentals and Applications, Springer, 2006.

Additional Readings:

A. Yamamoto, Organotransition metal chemistry, Wiley, 1986.

CHEMISTRY – 302: ORGANIC CHEMISTRY – III
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT – I: Reagents in Organic Synthesis:
Use of following reagents in organic synthesis and functional group transformations; Complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium disopropylamide (LDA), dicyclohexylcarboimide, 1,3-Dithiane (reactivity umpolung), trimethyl silyliodide, DDQ, DCC, DIBAL, Hoffmann – Loffler-Fretag, Miyamura, Stille, Negishi, Kamada Peterson synthesis Selenium dioxide and Baker yeast.

UNIT – II: Heterocyclic Chemistry
A) Synthesis and reactions of 5-membered heterocycles with one and two heteroatoms (Pyridine, imidazole, thiazole and pyrazole). Chichibabin and Shapiro reaction.
B) Diazines: Synthesis and general reactivity of pyridizine, pyrimidine and pyrazine.

UNIT – III: Green Chemistry: Introduction, the need of green chemistry, principles of green chemistry, Atom economy, E-factor, planning of green synthesis, tools of green chemistry (Solvents, reagents etc), Green reactions, Aldol condensation, Cannizaro reaction and Grignard reaction- comparison of the above with classical reactions-Green preparations, Applications phase transfer catalysts, Introduction to Microwave organic synthesis, Green alternatives to some common reactions, Industrial synthesis of Ibuprofen. Biodegradable polymers and plastics

UNIT – IV: Chemistry of Natural Products: A) Terpenoids and Carotenoids: Structure determination, stereochemistry biosynthesis and synthesis of the following representative molecules: geraniol, α-Terpenol, Menthol and β-Carotene**. B) Alkaloids**: Structure, stereochemistry, synthesis of following: Morphine, Ephedrine (±), Quinine, **C) Steroids:** Occurrence, nomenclature, basic skeleton, Diels hydrocarbon and study of the following: Cholesterol (natural synthesis), Hormones: Testosterone, Estrone, Progesterone.

UNIT – V: Biogenesis:
A). **Lipids:** Essential Fatty acids. Role of lipids in life processes: Significance of stereochemistry in fats, essential fatty acids, membranes / phospholipids. **B) Peptides and Protein**: Chemical and enzymatic hydrolysis of proteins, Peptides, amino acid sequencing. Merrifield Resin synthesis. **C) Enzymes:** Mechanism of Enzyme Action, examples of some typical enzyme mechanisms for chymotrypsin, lysozyme **D) Nucleic acids**: Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA) double helix model of DNA and its importance. Chemical and enzymatic hydrolysis of nucleic acids. Overview of replication of DNA, transcription RNA and genetic code.

Essential reading:

1. L.A. Paquette-Modern Heterocyuclic Chemistry, W.A. Benzamin Inc., 1968.
2. L. Finar, Organic Chemistry, Vol.II ELBS, 1986.
3. Green chemistry, ***V.K.Ahluwalia***, Ane book.
4. P.T. Anastas and J.C.Warner ***Green chemistry***, , Oxford
5. E.E. Cohn and P.K. Stumpf, Outlines of Biochemistry, Wiley Eastern, 1987.
6. H.R. Mahaler and E.H. Cordes, Biological Chemistry, Harper International, 1989.
7. Van Der Plas, Ring Transformation of Heterocyclics, Vol.I &II, Academic press, 1976.
8. T.L. Gilchrist, Heterocyclic Chemistry, Longman, 1989.

Additional reading:

1. Robert F. Weavwer, Molecular Biology, McGraw Hill, New Delhi, 1999.
2. Lubert Stryer, Biochemistry, Freeman, USA, 1989.
3. Michael B. Smith, Organic Synthesis, McGraw Hill, 1994.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, OUP, New Delhi, 2001.
5. Albert L.Lehninger, David L. Nelson, Michael M. Cox, Principles of Biochemistry, CBS, 2nd Edn. 1999.

CHEMISTRY – 303 : PHYSICAL CHEMISTRY – III
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT – I : Statistical Thermodynamics : Part – I

Thermodynamic probability and entropy, Ensembles – Postulates of ensemble averaging, canonical ensemble, grand canonical ensemble, micro canonical ensemble and their thermodynamics. Partition Functions – General relations for independent distinguishable and indistinguishable molecules (Boltzmann statistics), derivation and evaluation of translational partition function n using particle in a box model for ideal gases, derivation and evaluation of rotational partition function using rigid rotator model for ideal diatomic molecules, rotational partition function for linear and non-linear molecules (derivation not required).

UNIT – II : Statistical Thermodynamics : Part – 2

Derivation and evaluation of vibrational partition function for ideal diatomic gases using harmonic oscillator model, electronic partition function. a) Chemical equilibria in ideal gases : Reference state of zero energy for calculation of partition function of a system, expression for equilibrium constant in terms of partition functions, applications to some chemical equilibria. b) Some illustrations: Equations of state for ideal gases, Theories of specific heat capacity for solids (Einstein's model), ideal lattice gas (Langmuir absorption isotherm) theory of absolute reaction rates.

UNIT – III : Statistical Thermodynamics : Part – 3

Maxwell- Boltzmann statistics, Fermi-Dirac statistics, ideal Fermi-Dirac gas (Electrons in metals). Bose-Einstein statistics, ideal Bose-Einstein gas (helium). Statistical mechanics of imperfect gases, derivation of the virial equation of state for a ono-component gas, siginificance of virial coefficients, evaluation of second virial coefficient.

UNIT – IV : Macromolecules :

Average molecular weights – number average and weight average molecular weights, determination of molecular weights (viscosity, osomotic pressure, light scattering and sedimentation methods). polymerization reaction-free radical mechanisms, rates of polymerization reaction, cationic, anionic and emulsion polymerization in solution, optical and geometrical isomerism.

UNIT – V : Reactions on Surfaces :

Simple Langmuir isotherm (adsorption with dissociation, competitive adsorption) statistical treatment of ideal adsorption and non-ideal adsorption, chemical reactions on surfaces (General discussion, Unimolecular surface reactions-inhibition and activation energies. Biomolecular surface reactions two adsorbed molecules, one adsorbed molecule and a gas molecule, two gases adsorbed inhibition, example of C_2H_4 –H_2.

Suggested readings:

1. T. L. Hill Statistical Thermodynamics Addision Wesley 1960
2. D.A. Mcquarie Statistical Thermodynamics , Viva Books Pvt Ltd 2003
3. JM Seddon and JD Gale Thermodynamical and statistical mechanics RSC 2001
4. LK Nash Elements of Classical and statistical thermodynamics Addision –wesley 1970
5. M. C. Gupta Statistical Thermodynamics WEL 1995
6. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
7. K.J.Laidler Chemical Kinetics Harper and Row

Additional reading:

1. Principles of Polymer Science P.Bahadur, N.V.Sastry Narosa 2002
2. An introduction to Statistical Thermodynamics Robert H Gasser, N. Graham Richards WSC, 1995
3. J Raja Ram and JC Kuriakose Kinetics and mechanism of Chemical transformations McMillan 1993

CHEMISTRY – 304: APPLICATIONS OF SPECTROSCOPIC METHODS
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

Part A: INORGANIC CHEMISTRY (30+10)

Unit-I : Infrared and Raman spectroscopy: Structural studies involving IR and Raman Spectroscopy of coordination compounds containing the following molecules/ions and ligands. NH_3, H_2O, OH, SO_4^{-2}, ClO_4^-, COO^-, NO_2, CN^-, SCN^-, NO, O_2, PR_3, Halides, DMSO, azopyridine, oxime, quinine, acetylacetone, aminoacids.
Optical Electronic spectroscopy of metal complexes: Structural elucidation (cis, trans etc.). Calculation of 10Dq values. Interpretation of spectral bands of octahedral and tetrahedral metal complexes.

Unit – II : Magnetic Resonance Spectroscopy:
Electron spin resonance spectroscopy: ESR of d^1 and d^9 transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constants.
Nuclear magnetic resonance spectroscopy: Applications of ^{13}C, ^{1}H, ^{31}P and ^{19}F NMR spectroscopy in the structural assessment of inorganic compounds.

Unit – III : Mass Spectroscopy :
Principle of electron-impact induced mass spectrometry and FAB, qualitative and semiquantitative theories including QET, concept of metastable ions transitions, Stevensons's rules. Applications to metal compounds containing carbonyl, alkyl, cyclopentadienyl and acetylacetonate.
Mossbauer Spectroscopy: Principle, Isomershift, Quadrupole effect, effect of magnetic field, application to iron and tin compounds.

Part B: ORGANIC CHEMISTRY Max Marks (45+15)
(Unit I carries 12 marks and other Units 11 marks)

Unit I:
i) MASS SPECTROMETRY:
Introduction, ion production- EI, CI, FD and FAB factors affecting fragmentation, ion analysis, ion abundance
Mass spectral fragmentation of organic compounds: common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. Structure determination.

ii) ULTRAVIOLET AND VISIBLE SPECTROSCOPY:
Various electronic transitions (185-800nm), effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes and conjugated polyenes. Fiser – Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

Unit II: INFRARED SPECTROSCOPY:
Characteristics vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of different functional groups. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.

Unit III: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY - I
Continuous wave (CW) NMR spectroscopy, Fourier-Transform (FT) NMR spectroscopy, Chemical shift in NMR spectroscopy and determination of organic structure from spectra, spin-spin coupling, shielding mechanism, rules of spectral analysis, virtual coupling, hindered rotation, karplus curve-variation of coupling constant with dihedral angle, simplification of complex spectra, nuclear magnetic double resonance, solvent- induce shifts, The effect of chirality, nuclear overhauser effect (NOE) and its applications.

Unit IV: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY - II
A) ^{13}C NMR SPECTROSCOPY: General consideration, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon) coupling constants. The applications of multipulse techniques like INEPT, DEPT, DEPTQ. Spin decoupling methods – homonuclear and heteronuclear decoupling.
B) 2D NMR Spectroscopy – 2D NMR, the spectra of the "other nuclei", Correlations through chemical bonds: Homonuclear and heteronuclear spin correlation- COSY 90 and COSY 45- their applications, NMR spectral analysis from COSY (problems), NOESY- Interpretation of stereochemistry of organic molecules.
C) Elucidation of structure of organic compounds from UV-Visible, IR, NMR and MS Data.

Essential reading:

1. Kemp, Organic Spectroscopy, 3rd Edn, MacMillan, Hong Kong, 1991.
2. D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, 4th Edn. Tata McGraw-Hill, New Delhi, 1991.
3. D. L. Pavia, G. M. Lampman and G. S. Kriz, Introduction to Spectroscopy, 3rd Edn. Harcourt College Publishers, 2007.
4. R. M. Silverstein and F. Webster, Spectroscopic Identification of Organic Compounds, 6th Edn. John Wiely, New York, 1998.
5. K. Beimann, Mass Spectroscopy-Application to Organic Chemistry, McGraw-Hill, New York, 1962.
6. J. Barker, Mass Spectroscopy, 2nd Edn. John Wiely, New York, 2000.
7. K. Nakamato, IR and Raman Spectra of Inorganic and Coordination Compounds, 4th Edn. John Wiley, 1986.
8. R. S. Drago, Physical Methods in Chemistry, Saunders College Publishers, 1977.
9. M. R. Litzow and T R Spelding, Mass Spectroscopy of Inorganic & Organometallic Compounds, Elsevier,73

Additional reading:

1. A.B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Edn. Elsevier.
2. J. R. Dyer, Application of Adsorption Spectroscopy of Organic Compounds, 2nd print, Prentice-Hall, New Jersey, 1971.
3. H. Duddeck and W. Dietrich, Structure Elucidation by Modern NMR A Workbook, 2nd revised and enlarged edition. Springer-Verlag, New York, 1992

4.

CHEMISTRY – 305 : LABORATORY COURSE IN PHYSICAL CHEMISTRY
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

1. Determination of equilibrium constant of the reaction KI +
2. Determination of energy of activation for hydrolysis of an ester, using an acid catalyst.
3. Study of the reaction between acetone and iodine in the presence of an acid.
4. Determination of the partial molal volume of a solute in solution.
5. Determination of molecular weight of a non-electrolyte\electrolyte by cryoscopy.
6. Determination of dissociation constant of a weak electrolyte conductometrically and verification of Ostwald's dilution law.
7. Determination of specific rotation ofr source and rate constant of its hydrolysis, using a polarimeter.
8. Solubility curve for a ternary system of liquids (water acetic acid chloroform).
9. To obtain the phase diagram for a two component system forming a congruent compound (benzophenone-diphenylamine).
10. Determination of transport number of ions by Hittorf's method.
11. Determination of strengths of strong and weak acids in a given mixture , using the pH meter.
12. Determination of a) cell constant b) strengths of strong and weak acids in a given mixture, conductometrically.
13. Determination of the order of saponifrication for the reaction of ethyl acetate with sodium hydroxide, conductometrically.
14. Determination of the order of saponification for the reaction of ethyl acetate with sodium hydroxide, conductometrically.
15. Determination of the equivalent conductivity of strong electrolytes at different dilutions (HCl, NaCl,
16. CH_3 COONa) and hence to determine the equivalent conductivity of a weak electrolyte (CHCOOH) at infinite dilution.
17. Determination of solubility and solubility product of sparingly soluble salts ($PbSO_4$ and $BaSO_4$), conductometrically.
18. Determination of strengths of halide4s in a mixture, potentiometrically.
19. Determination of the valency of mercurous ions, potentiometrically.
20. Determination of the hydrolysis constant of ammonium chloride and the dissociation constant of ammonium hydroxide potentiometrically.
21. Determination of the dipole moment of a polar molecule 7usinhg the dipole meter.
22. Determination of phase transition temperature through differential thermal analysis.
23. Determination of glass transition temperature of a given salt, conductometrically.
24. Determination of the PK of an indicator spectrophotometrically.
25. Determination of the PK of the indicator in micelle medium sepcttophotometrically.
26. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide. Studying the kinetics as an iodine-clock reactions.
27. Determination of the composition and the stability constant of a complex, spectrophotometrically.

Suggested reading:

1. Experiments in Physical Chemistry J.C.Ghosh Bharati Bhavan 1974,New Delhi
2. Advanced experimental chemistry (Physical) J.N.Gurtu, & NR Kapoor, S.C. Company 1980
3. Laboratory manual in Physical chemistry WJ Popiel, ELBS 1970
4. Advanced Practical in Physical Chemstry JB Yadav, Pragati prakasan Meerut
5. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman.

Additional reading

6. Findley's practical Physical Chemistry, B. P. Levitt, Longman.
7. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill.

CHEMISTRY – 401: ANALYTICAL AND COMPUTATIONAL CHEMISTRY
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

Unit - I: Purification and Separation Techniques
Normal and reversed phase liquid chromatography, partition, adsorption, and ion exchange chromatography, gas chromatography, high performance liquid chromatography. Hyphenated technique e. g. GC-MS, HPLC-ICPMS

Unit -II: Electrochemical methods of analysis:
Polarography: Linear scan polarography, Dropping mercury electrode (DME), Ilkovic equation. Voltammetry: Hydrodynamic voltammetry, amperometry, cyclic voltammetry, Coulometry and their applications.

Unit -III: Thermal and Nuclear methods of analysis:
Thermal methods of analysis: Thermogravimetry (TG), Differential thermal analysis (DTA), Differential Scanning Calorometry (DSC): Principles, instrumentation, applications.
Nuclear methods of analysis: Neutron activation analysis (NAA) and X-ray Fluorescence spectroscopy (XRF): Principles, instrumentation, applications. Atomic absorption spectroscopy (AAS): Principles, instrumentation, methodology and applications.

Unit IV: Introduction to computer and computing:
Basic structure and functioning of a computer (with demonstration), Algorithm, Flowchart, Development of small computer codes (in FORTRAN or C) involving simple formula in chemistry such as van der Waal's equation, pH, kinetics and radioactive decay.

Unit V: Concepts in Computational Chemistry:
Scope of computational chemistry, Potential energy surface, Force fields, concept of Basis set (STO-3G, 3-21G, 6-31G, 6-31G*, 6-31G**), The Born-Oppenheimer approximation, potential energy surfaces, local and global minima, Hartree-Fock approximation, Kohn-Sham Equation and Density Functional Theory.
(Demonstration of the key concepts using suitable software package)

Essential Reading:

1. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W.B. Saunders.
2. Analytical Chemistry-Principles, J. H. Kennedy, W.B. Saunders.
3. Analytical Chemistry-Principles and Techniques, .G. Hargis, Prentice Hall.
4. Principles of Instrumental Analysis, D.A. Skoog, W. B. Saunders.
5. Instrumental methods of chemical analysis by B K Sharma Goel publishing House Ltd
6. Essentials of Nuclear chemistry HJ Arnikar, Wiley eastern.
7. D. A. McQuarrie, *Quantum Chemistry* (University Science Books, Mill Valley, CA,).
8. P. W. Atkins. *Molecular Quantum Mechanics*, Oxford Univ. Press

Suggested Reading:

1. Analytical chemistry, G.D. Christian, J. Wiley.
2. Quantitative Analysis, R. A. Day, Jr. and A.L. Underwood, Prentice Hall.
3. Environmental Solution Analysis, S. M. Khopkar, Wiley Eastern.
4. Basics Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
5. Handbook of Instrumental Techniques for Analytical Chemistry, F.Settle, Prentice Hall.
6. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders.
7. Analytical chemistry of macroscopic and supramolecular compounds S M Khopkar, Narosa 2002.
8. Christopher J. Cramer, *Essentials of Computational Chemistry: Theories andModels*, 2nd Ed. Wiley & Sons, New York

Chemistry CH – 402: CHEMISTRY OF ADVANCED MATERIALS
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

Unit- I: **Introduction to Nanomaterials:**

Introduction - definition of nanoscience, nanochemistry -classification of the nanomaterials – zero dimensional nano structures - one dimensional nanostructures – nanowires, nanorods and nano tubes– two dimensional nanostructures – thin-films– three dimensional nanostructures – quantum dots, fullerenes and dendrimers. Synthesis of Nanomaterials: Sol-gel and CVD

Unit- II: **Properties of nanomaterials:**

Basic properties and Measuring Methods: Particle size, particle shape, particle density, melting point, specific surface area and pore, crystal structure, surface characterization, Elementary ideas of electrical properties, electrochemical, thermo-physical properties, optical properties, magnetic properties, catalytic properties. Few selective examples of recent emerging applications: Solar cell, Fuel cell, nanoecotoxicology.

Unit -III: **Chemistry of Mesogens:**

Introduction - Difference between liquid crystal, solid and liquid. Order parameters, Classification of liquid crystals. Thermotropic liquid crystals, nematic, cholestreric and smectic mesophases. Lyotropic liquid crystals, constituents of lyotropic liquid crystals, structures of lyotropic liquid crystal phases, biological membranes. Important applications of liquid crystals.

Unit- IV: Pharmaceutical Chemistry

Concept and definition of Pharmacophore, Drug Discovery, Design and Development. Structure-activity relationships: Strategies in drug design. QSAR and combinatorial synthesis. Optimization of drug-target interactions and access to drug targets. ADMET of drugs. Pro-drugs and drug delivery systems. Elementary ideas on Nanomedicines. Biomimicking systems: Cyclodextrins as enzyme mimics, ion channel mimics.

Unit- V: Applications of Supramolecule:

Molecular sensors: Electrochemical and optical sensors, Switches and molecular machinery, Photochemical devices, MRI contrast, Anti cancer agents, Cosmetics and food industries.

Suggested Books

1. Supramolecular Chemistry, Paul D Beer, Philip A. Gale and David K. Smith
2. Supramolecular Chemistry-Fundamentals and Applications, katsukiko Ariga and Toyaki Kunitake
3. Introduction to Supramolecular Chemistry, Helena Dodziuk
4. Liquid Crystals by S. Chandrasekhar.
5. Thermotropic Liquid Crystals by Vertogen and Jeu

Essential Readings:

1. Introduction to Nanoscale science and Technology, (Ed) Massimiliano Di Ventra, Kluwer Academic.
2. Nanomaterials CNR Rao, Wiley-VCH
3. M.J.O.Connell, Carbon Nanotubes: Properties and Application, CRC Press, 2006
4. Nanostructures and Nanomaterials,Synthesis, Properties Applications, by G.Cao, Imperial College Press, 57 Shelton Street, Covent Garden, London WC2H 9HE, 2004
5. C.N.R.Rao, A.Muller, A.K.Cheetham, Nanomaterial Chemistry: Recent developments and new directions, Wiley, 2007.
6. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill, New Delhi, 2007.
7. Nanoparticle Technology Handbook, Masuo Hosokawa, Kiyoshi Nogi, Makio Naito, Toyokazu Yokoyama, Elsevier 2007
8. Yury Gogotsi , Nanomaterials Handbook, CRC press, 2008

Suggested Readings :

1. J.W.steed, D.R.Turner, K.Wallace, Core Concept in Supramolecular Chemistry and Nanochemistry, Wiley, 2007
2. H.S. Nalwa, Handbook of Nanostructured Materials and Nanotechnology, Academic Press, 2000.
3. M.S. Dresselhaus, G. Dresslhous, P.C. Eklund, Science of Fullerenes and Carbon Nanotubes, Academic Press, San Diego, USA, 1996.
4. M.S. Dresselhaus, G. Dresslhous, P. Avouris, Carbon Nanotubes: Synthesis, Structure, Properties and Application, Springer, Berlin, Germany, 2001.
5. P. J. Bruke, Nanotubes and Nanowires, Spring, 2004
6. Advanced semiconductor and organic nano technique part I, II, III Hadis Morkoc, Elsevier
7. Biofunctionalization of nanomaterials Challa SSR Kumar Wiley-VCH
8. J.A.Rodriguez, M.F.Garcia, Synthesis, properties and application of oxides Nanomaterials, Wiley, 2007

CHEMISTRY – 403 A: INORGANIC CHEMISTRY – IV
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional: 25, Pass Marks:10

UNIT – I: Organometallic Chemistry
Synthesis, structure, bonding (qualitative treatment only) and reactivity of Metal – Carbon Multiple bond: Alkylidenes, Alkylidynes. π-Coordination of C-C multiple bonds: Alkyne, Di and Polyenes, Allenes, Alkynes, Carbocyclic Polyene ligands: Allyls, Pentadienyls, Cyclopropenyls, Cyclobutadienes, Ferrocene, Arenes. Multidecker sandwitch compounds.

UNIT – II: Photochemistry of metal complexes:
Excited states and excited state processes **:** Ligand field states, charge transfer states, thexi and DOSENCO states, photophysical processes (radiative and nonradiative transitions). Photochemical reactions: L-F excited states and Cr(III) complexes, LMCT states and MLCT states. Survey of photoreactions of complexes of d-transitions elements. Applications of photochemical reactions of coordination compounds: Synthesis and catalysis chemical actinometry photochromism.

UNIT – III: Radiochemical method of analysis:
Tracers in chemical analysis. The tracer technique, isotopic exchange and other tracer reactiobns, analytical applications, Hot atom chemistry. Methods of radiochemical separation: Carriers, precipitation, ion-exchange, solvent extraction, electrochemical method isotope dilution technique and its applications.

UNIT – IV: Bioinorganic chemistry:
Copper: Ceruloplasmin, cytochrome oxidase and superoxide dismutase, Tyrosine. Cobalt: carbonic anhydrase, carboxy peptidase and metallothioneins, interchangeability of zinc and cobalt in enzymes. Magnesium, : Complexes with ATP and ADP, active transport of ions across membrane, Catalase and calcium in living cell and transport and regulation. Metal ion detoxification.

UNIT – V: Design and Synthesis of ligands and complexes.
Ligand design and synthesis: Schiffbase, oxime, azo, macrocycle, tripod, podand, coronand, cryptand. Coordination compound design and synthesis: Self-assembly, Structure directed synthesis, building block, metalloligand, supramolecular framework.
Crystal Engineering: Crystal Design Strategies, crystallization and crystal growth, Polymorphism, Coordination polymers.

Essential Readings:

1. H. J. Emeleus and A. G. Sharpe, Modern Aspects of inorganic chemistry, 4th Edn. Rout ledge and Kegan Paul, London, 1973.
2. R. W. Hay, Bio-Inorganic Chemistry, Halsted Press, 1984.
3. F. wells, Structural Inorganic Chemistry, 5th Edn. OUP, Oxford, 1984.
4. W. E. Addison, Structural Principles in Inorganic Compounds, Longmans, London, 1974.
5. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books.
6. G. R. Desiraju, J. J. Vittal and A. Ramanan, Crystal Engineering, IISC Press, World Scientific, 2011.

Suggested Reading:

1. J. M. Lehn, Supramolecular Chemistry, VCH.
2. R. C. Mehrotra and A. Singh, Organo-metallic Chemistry, New Age International.
3. R. West, Solid State Chemistry and its Application, Wiley, New York, 1984.
4. E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, Blackwell
5. Scientific Publishers, Oxford, 1987.

6. D. M. Adams, Inorganic Solids, Wiley-Interscience, New York, 1974

CHEMISTRY – 403 B: ORGANIC CHEMISTRY – IV
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT – I: A) Organometallic Chemistry:
Bonding of transition metal in organo-metallic complexes. Fluxionality, epolarization of reactive or unstable molecules. Insertion reactions. Formation of C-C bonds with the aid of organo-Ti, Ce, B, Si and Zn compounds and their stereochemical or chemoselective applications. Role of organo-Cd, Hg and Pd compounds in organic synthesis.
B) Ylids: Phosphorous, Nitrogen and Sulphur Ylids and stereochemistry of compounds containing Phosphrous, Sulfur and Nitrogen.

UNIT – II: Disconnection Approach (Retro Synthesis): An introduction to Synthons and synthetic equivalents, disconnection approach,functional group interconversions. One group C-X and two group disconnections in 1,2,1,3 - ,1,4-& 1,5- difunctional compounds , Retro- synthesis of Alkene ,acetylenes and aliphatic nitro Alcohols and carbonyl compounds, amines , the importance of the order of events in organic synthesis, chemoselectivity, regioselectivity. Diels Alder reaction, Michael addition and Robinson annulation. Retro- synthesis of aromatic Heterocycles and 3, 4, 5 and 6 membered carbocyclic and heterocyclic rings. Reversal of polarity (Umpolung). Retro synthesis of Camphor and Longifolene

UNIT –III: Heterocyclic Synthesis-:
Reactions of pyridine quinoline & isoquinoline, Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions. b) Benzo-Fused Five Membered Heterocycles: Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes. c) Six-membered heterocycles with two or more heteroatoms: Synthesis and reactions of triazines, tetrazines and thiazines.

UNIT – IV: Medicinal Chemistry-I: Chemistry of Drug Design
A) Development of new drugs, procedures followed in drug design, concepts of prodrugs and soft drugs. Theories of drug activity, Quantitative structure activity relationship (QSAR). Elementary treatment of drug receptor interactions, Structure-Based Drug Design, Transporters and Enzymes as drug targets, Lipophilicity, LD-50, (Mathematical derivations of equations excluded).

UNIT – V: Medicinal Chemistry-II: Application
A) Study of the Following types of drugs: (No synthesis is required unless mentioned).
i) Antibiotics: Preparation or synthesis of semi synthetic penicillin, conversion of penicillin into cephalosporin, general account (synthesis is excluded) of tetracycline & macrocyclic antibiotics
ii) Antimalerials: Trimethoprim.
B) Anti-neoplastic drugs: Cancer chemotherapy, Treatment schemes, pharmacokinetics/pharmacodynamics and mode of action of mechloraethamine, cyclophosphamide, structure and role of Mephalan, uracils, mustards, Study of the role of (i)Flavones: Tangeritin (synthesis is not required), Vinca Alkoloids: Vincristine (synthesis is not required) Study of the recent developments in cancer chemotherapy viz., Photodynamic Therapy (PDT).

Essential reading:

1. F. Hill, Organotransition Metal Chemistry, Royal Society of Chemistry, 2002.
2. R. C. Mehrotra and A. Singh, Organometallic Chemistry: A unified approach, 2nd Edn., New Age International Pvt. Ltd, New Delhi, 2000.
3. J. Pearson, Metalloorganic Chemistry, John Wiely, 1985.
4. R. E. Ireland, Organic Synthesis, Prentice-Hall, 1969
5. K. C. Nicholson and E. J. Sorenson, Classics in Total Synthesis, VCH, 1996.
6. E.E. Cohn and P.K. Stumf, Outlines of Biochemistry, Wiley Eastern, 1987.
7. J.D. Bulock, The Biosynthesis of Natural products, McGraw Hill, New Delhi, 1986.
8. T.L. Gilchrist, Heterocyclic Chemistry, Longman, 1989.
9. Jould and Mills, Heterocyclic Chemistry, Blackwell, 1988.
10. Alka L.gupta, "***Medicinal Chemistry***," Pragati Prakasan Meerut.
11. AhluwaliaV.K.,MaduChopra "***Medicinal Chemistry***," Ane books.

Additional reading:

1. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Parts A and B, Plenum Press, 1990.
2. Robert F. Weaaver, Molecular Biology, 1999, McGraw Hill New Delhi.
3. Lubert Stryer, Biochemistry, 1989, Freeman, USA.
4. Albert L. Lehninger, David L. Nelson, Michael M. Cox, Principles of Biochemistry, CBS Publishers and Distributors, 2nd Edn.1999.

CHEMISTRY – 403C : PHYSICAL CHEMISTRY – IV
Max. Marks: 100, External: 75, Pass Marks: 30, Sessional:25, Pass Marks:10

UNIT – I : Photophysical Processes in Excited State:

Types of photophysical pathways, Radiationless transitions, Fluorescence emission, Triplet state and phosphorescence emission, Fluorescence quenching, Stern-Volmer equation, Concentration quenching and excimer formation, Quenching by foreign substrates, Exciplex formation.

UNIT – II: Solvent and Environmental Effects on Fluorescence:

Solvent polarity effect; Derivation and application of Lipper-Mataga (LM) equation, effect of viscosity, temperature effects; Additional factors that effect fluorescence emission; effect of solvent mixtures: specific and non-specific interactions.
Biochemical applications of environment sensitive fluorescent probes.

UNIT – III : Solid State :

a) Physical properties of solids : i) Thermoelectric effects : Thomson, Peltier. Seebeck and Hall effects, dielectric materials, ferro-pyro and piezo electricity and its applications. Ii) Optical properties ; absorption, photoconductivity and luminescence. B) Electrically conducting organic solids : Organic metals, conjugated systems, electrically conducting polymers, organic charge-transfer complexes, organic super conductors.

UNIT – IV : Liquid State :

Cohesion of liquids and internal pressure, intermolecular forces and pair potential functions – hardsphere and Lennard-Jones potential functions. Partition function for liquids : Classical partition function, cell theory of liquids considering hard-sphere potential function, concept of communal energy and communal entropy, radial distribution function method for liquids : Clausius virial theorem, equation of state in terms of radial distribution function.

UNIT – V: Chemical Dynamics:

Dynamics of gas phase reactions: : Hydrogen-bromine reaction, pyrolysis of hydrocarbons, pyrolysis of acetaldehyde, decomposition of ozone, decomposition of nitrogen pentoxide. Dynamic of unimolecular reactions, Lindemann-Hinshelwood and the Rice-Ramsperger-assel-Marcus (RRKM) theories of unimolecular reactions, chemical reaction dynamics, steady state kinetics, kinetic and thermodynamic control of reactions.

Essential reading:

1. Physical chemistry, P.W. Atkins, 7th edn 2000, OUP
2. Rastogi and Mishra an introduction Chemical Thermodynamics, VPH, 1980
3. Liquid state Pryde, Hutchinson&co 1966
4. Solid state chemistry ARWest,
5. Chemical Kinetics, K. J. Laidler, McGraw Hill.
6. Foundation of chemical Kinetics S. W. Benson MGH, 1982

Suggested reading:

1. Theoretical electrochemistry Antropov Mir Publishers 1980
2. Kinetics and Mechanism of Chemical Transformations, J. Rajaram and J.Kuriacose, McMillan.
3. Micelles, Theoretical and applied Aspects, V. Moroi, Plenum.
4. Modern Electrochemistry Vol. I and Vol. II, J.O.M., Bockris and A.K.N. Reddy, Plenum.
5. Theoretical electrochemistry, Glasstone, AEN 1960

Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

Chemistry CH – 404: Project Work
Max. Marks: 200, External: 150, Pass Marks: 60, Sessional:50, Pass Marks:20

Project Work : A/B/C

A = Inorganic

B = Organic

C = Physical

Consolidation of all changes brought about in the MSc (Chemistry) Syllabus
(Proposed to be effective from 2013-14 Session)

CH-101 Inorganic Chemistry-I

	Addition	**Deletion**
Unit II	MO treatment of simple diatomic (homo & hetero) system with special reference toB_2, C_2, N_2, F_2, CO, HCl etc.	-
Unit III	Rearrange	-
Unit IV	C budget, C-credit, CO_2 sequestration, SO_x, Photochemical Smog (PS) and chemistry of PS formation, Sulphurous Smog. biological defense mechanism	-
Unit V	(concept, examples, techniques of detection)	-
Suggested Reading,	9. G. L. Miessler and D. A. Tarr, inorganic Chemistry, Pearson. 2009;10. J. D. Lee, Concise Inorganic Chemistry, Chapman & Hall Ltd.,1991; 11. G. Wulfsberg, Inorganic Chemistry, Viva Books Pvt. Ltd. 2002.; 12. A. K. Das, Fundamental concepts of inorganic chemistry, Vol III, Second Edn. CBS, 2010.; 13. G. N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, U. N. Dhar & Sons Pvt. Ltd.1993;14. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry-Principles of Structure and Reactivity, Addison –Wesley Publishing Company, 1993	-

CH-102 Organic Chemistry-I

Unit No	**Addition/Modification**	**Deletion**
1	Same as earlier	
2	Methods of asymmetric synthesis including chiral pool, chiral auxiliary, chiral reagents; enantio and diastereo selective and specific synthesis. Inclusive of substrate control and reagent control strategies eg, Sharpless epoxidation and di-hydroxylations with AD-mix-□ and □.	Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus. Novel methods of asymmetric synthesis including enzymatic and catalytic nexus, enantio and diastereo selective synthesis
3	SNi along with mixed SN^1 and SN^2 and SET mechanisms	The ortho/para ratio, orientation in other ring systems
4	Enolates, emines and enamines: their roles in chemoselective and regioselective C-C bond formations. Alkylation of enolates, emines and enamines and their stereochemical outcomes.	Carboxylic acid derivatives and decarboxylation reactions
5	stereochemical aspects including Cram's rule. 6-membered cyclic substrate. Pyrolytic syn-Elimination reactions of esters, xanthates and sulfoxides	Addition to cyclopropane ring, hydrogenation of double and triple bonds and hydrogenation of aromatic rings. Leaving groups including biological

CH-103 Physical Chemistry-I

Name of the Unit	**Modification**

UNIT-I	Rearranged
UNIT-II	Rearranged, Debye-Huckel Theory has been shifted to Unit –I (CH-204)

CH-104 Quantum Chemistry and Chemical Bonding

Name of the Unit	Modification
UNIT-I	Rearranged
UNIT-II	Rearranged, Roothan's solution has been added

CH-201 Inorganic Chemistry-II

	Addition	Deletion
Unit I	-	Mechanism of exchange reactions, Bleaney-Bowers equation
Unit II	Charge-transfer transitions of inorganic coordination compounds (different type).	-
Suggested Reading	6. Asim K. Das, Bioinorganic Chemistry, Books & Allied (P) Ltd., Kolkata 7. P K Bhattacharya, Metal ions in Biochemistry, Narosa, New Delhi 8. N. Gupta, and Monal Singh, Essential of Bio-inorganic chemistry, Pragati Prakashan.	-

CH-202 Organic Chemistry-II

Unit No	Addition/Modification	Deletion
1	Same as earlier	
2	Same as earlier	
3	Pinacol-pinacolone, Tiffeneau-Demjanov; Phosphorous, nitrogen and sulphur ylides.	Acyl Cations, PPA cyclization, Carbenoids
4	Allylic hydrogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, Sandmeyers reaction and Hunsdiecker reaction, photo-dissociation, gas phase photolysis, photochemistry of alkynes, intramolecular reactions of the olefinic bonds, geometrical isomerism, rearragements of 1,4 (di-pi-methane) and 1,5 dienes, photochemistry of carbonyl compounds including Patterno Buchi (oxitane formation) , Norrish Types I and II (intramolecular reactions of carbonyl compounds) intermolecular cycloaddition reactions and photochemistry of aromatic compounds,	c) Retro synthesis, introduction, synthons, protecting groups, disconnection protocols one group C-C (alcohols, carbonyls) two groups C-C Diels-Alder reaction, Michael addition, Retro synthesis of Camphor and Longifolene.
5	Same as earlier	

CH-203 MOLECULAR SPECTROSCOPY

Name of the Unit	Modification
UNIT-I	Rearranged
UNIT-III	Rearranged

CH-204: PHYSICAL CHEMISTRY-II

Name of the Unit	Modification
UNIT-I	Rearranged
UNIT-V	Rearranged, Kinetics of micelle formation has been added

CH-205: LABORATORY COURSE IN ORGANIC CHEMISTRY

Restructuring of the experiments

Inclusion of -- Use of Computer in organic chemistry: Simple operations like Drawing of structures, Optimization etc

CH-301 Inorganic Chemistry-III

	Addition	Deletion
Unit IV		Nuclear reactions on stars
Suggested reading	5. J. M. lehn, Supramolecular Chemistry- Concepts and Perspectives, VCH, Winheim, 1995 6. P. D. Beer, P. A. Gale and D K. Smith, Supramolecular Chemistry, Oxford Scince Publications, 1999 7. K. Ariga and T. Kunitake, Supramolcular Chemistry,- Fundamentals and Applications, Springer.2006	-

CH-302 Organic Chemistry-II

Unit No	Addition/Modification	Deletion
1	Same as earlier	
2	Hoffmann – Loffler-Fretag, Miyamura, Stille, Negishi, Kamada Peterson synthesis	
3		Introduction of 3- and 4- membered Heterocycles**:** Aziridine, thiirane, Oxetane Azetidine, Thietane & their derivatives & Reactions and β-Lactum ring antibiotics
4	**Chemistry of Natural Products: A) Terpenoids and Carotenoids**: Structure determination, stereochemistry biosynthesis and synthesis of the following representative molecules: geraniol, α-Terpenol, Menthol and β-Carotene**. B) Alkaloids**: Structure, stereochemistry, synthesis of following: Morphine, Ephedrine (±), Quinine, **C) Steroids:** Occurrence, nomenclature, basic skeleton, Diels hydrocarbon and study of the following: Cholesterol (natural synthesis), Hormones: Testosterone, Estrone, Progesterone.	**Enzymes :** Introduction and historical perspective, biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Enzyme kinetics: Michaelis Menten and Lineweaver-Burk plots. b) Mechanism of Enzyme Action, examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease and lysozyme c) Terpenoids and Carotenoids: Structure determination, stereochemistry biosynthesis and synthesis of the following representative molecules: geraniol, A-Terpenol, Menthol and β-Carotene. d) Alkaloids: Structure, stereochemistry, synthesis of following: Ephedrine (±), Quinine and Reserpine.
5	**Biogenesis:** Rearranged	

CH – 304: APPLICATIONS OF SPECTROSCOPIC METHODS
Part B

Unit No	Addition/Modification	Deletion
1	**MASS SPECTROMETRY:** Introduction, ion production-EI, CI, FD and FAB factors affecting fragmentation, ion analysis, ion abundance, Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. Structure determination.	
2	Unchanged	
3	Continuous wave (CW) NMR spectroscopy, Fourier-Transform (FT) NMR spectroscopy, Chemical shift in NMR spectroscopy and determination of organic structure from spectra, spin-spin coupling, shielding mechanism, rules of spectral analysis, virtual coupling, hindered rotation, karplus curve-variation of coupling constant with dihedral angle, simplification of complex spectra, nuclear magnetic double resonance, solvent- induce shifts, The effect of chirality, nuclear overhauser effect (NOE) and its applications.	Chemical shift, spin-spin interaction, shielding mechanism, correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and oxygen and Nitrogen (alcohols, phenols, enols, carboxylic acids, amines and amides) chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling, stereochemistry, hindered rotation, karplus curve-variation of coupling constant with dihedral angle, simplification of complex spectranuclear magnetic double resonance, contact shift reagents, solvent effects, nuclear overhauser effect (NOE).

4	**^{13}C NMR SPECTROSCOPY: 1D continued**: General consideration, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon) coupling constants. The applications of multipulse techniques like INEPT, DEPT, DEPTQ. Spin decoupling methods – homonuclear and heteronuclear decoupling. **B) 2D NMR Spectroscopy** – 2D NMR, the spectra of the "other nuclei", Correlations through chemical bonds: Homonuclear and heteronuclear spin correlation- COSY 90 and COSY 45- their applications, NMR spectral analysis from COSY (problems), NOESY- Interpretation of stereochemistry of organic molecules. **C)** Elucidation of structure of organic compounds from UV-Visible, IR, NMR and MS Data.	**CARBON 13 NMR SPECTROSCOPY:** General consideration, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon) coupling constants. Two dimension NMR Spectroscopy – COSY, NOESY, DEPT techniques. Biological applications of NMR. **MASS SPECTROMETRY:** Introduction, ion production- EI, CI, FD and FAB factors affecting fragmentation, ion analysis, ion abundance, Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. Structure determination.

CH-403

CH-403 A : Inorganic Chemistry IV

	Addition	**Deletion**
Unit I	bonding (qualitative treatment only)	Vinylidenes
Unit IV	Metal ion detoxification	Sodium pump, biological defense mechanism
Unit V	Design and Synthesis of ligands and complexes: Azo; Crystal engineering: Crystal Design Strategies, crystallization and crystal growth, Polymorphism, Coordination polymers.	Synthetic methodology for transition and non-transition metal compounds**:** Polypyrine, ligand topology and moleculer mechanics, polymeric ensemble (chain, sheet network), molecular machine, biomodelling, molecular/crystal engineering
Suggested reading	6. G. R. Desiraju, J. J. Vittal and A. Ramanan, Crystal Engineering, IISC Press, World Scientific, 2011.	-

CH-403 B : Organic Chemistry IV

Unit No	**Addition/Modification**	**Deletion**
1	**B) Ylids:** Phosphorous, Nitrogen and Sulphur Ylids and stereochemistry of compounds containing Phosphrous, Sulfur and Nitrogen	
2	**Disconnection Approach (Retro Synthesis)** : An introduction to Synthons and synthetic equivalents, disconnection approach,functional group interconversions. One group C-X and two group disconnections in 1,2,1,3 - ,1,4-& 1,5- difunctional compounds , Retro- synthesis of Alkene ,acetylenes and aliphatic nitro Alcohols and carbonyl compounds, amines , the importance of the order of events in organic synthesis, chemoselectivity, regioselectivity. Diels Alder reaction, Michael addition and Robinson annulation. Retro- synthesis of aromatic Heterocycles and 3, 4, 5 and 6 membered carbocyclic and heterocyclic rings. Reversal of polarity (Umpolung). Retro synthesis of Camphor and Longifolene	Stereoelectronic effects in organic reactions, conformation and reactivity, Chemical and Stereochemical aspects of molecular recognization: Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors (host-guest interaction) and design principles. Cryptands, cyclophanes. Molecular self assembly.
3	**Heterocyclic Synthesis-:** Reactions of pyridine quinoline & isoquinoline, Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions. b) Benzo-Fused Five Membered Heterocycles: Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes. c) Six-membered heterocycles with two or more heteroatoms: Synthesis and reactions of triazines, tetrazines and thiazines.	**Natural products:** Introduction and classification based on biogenesis. Coenzyme and their role in biochemical transformations with reference to coenzyme A, lipoic acid, pyridoxal phosphate, thiamine pyrophosphate, tetrahydrofolic acid. Vitamin B12. Haemoglobin as oxygen carrier. Biosynthesis of Flavonoids-acetate and Shikimic acid path way

4	.**Medicinal Chemistry-I: Chemistry of *Drug Design*** A) Development of new drugs, procedures followed in drug design, concepts of prodrugs and soft drugs. Theories of drug activity, Quantitative structure activity relationship (QSAR). Elementary treatment of drug receptor interactions, Structure-Based Drug Design, Transporters and Enzymes as drug targets, Lipophilicity, LD-50, (Mathematical derivations of equations excluded).	**Polymer and Carbohydrates:** Biodegradable polymers and plastics. Chemical reagents and polymer bonding. Natural products derived from carbohydrates- sialic acides, vitamin C. O, S, N- glycosides. Cardiac glycosides, Digitoxin, Heparin. Saccharides as reagents and synthesis of chiral compounds. Concept and synthesis of Prostaglandin, cholesterol, linosterol, estrogens, progesterone and testosterone and their biological functions.
5	**Medicinal Chemistry-II: Application** A) Study of the Following types of drugs: (No synthesis is required unless mentioned). i) Antibiotics: Preparation or synthesis of semi synthetic penicillin, conversion of penicillin into cephalosporin, general account (synthesis is excluded) of tetracycline & macrocyclic antibiotics ii) Antimalerials: Trimethoprim. B) Anti-neoplastic drugs: Cancer chemotherapy, Treatment schemes, pharmacokinetics/pharmacodynamics and mode of action of mechloraethamine, cyclophosphamide, structure and role of Mephalan, uracils, mustards, Study of the role of (i)Flavones: Tangeritin (synthesis is not required), Vinca Alkoloids: Vincristine (synthesis is not required) Study of the recent developments in cancer chemotherapy viz., Photodynamic Therapy (PDT).	Development of new drugs (Preliminary concept on Bio-Chem informatics), procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and open drugs and enzyme inhibition drugs. Structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect. Theories of drug activity : Occupancy, rate, induced fit theory. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Lipophilicity, LD-50, (Mathematical derivations of equations excluded). Cancer chemotherapy - role of alkylating agents and plant products (Vinca alkaloids, flavones and flavonoids, taxol) in treatment of cancer. Function of cyclophosphamide, melphalan, uracil mustard and nitrosoureas as anti cancer drugs.

CH-403 (C): PHYSICAL CHEMISTRY-IV

Name of the Unit	Modification
UNIT-I	Electrochemistry and its application have been removed; Photophysical processes in excited state have been introduced.
UNIT-V	Dynamics in living systems has been removed; Solvent and environmentat effects on fluorescence have been introduced.
UNIT-II, III and IV	Now redesignated as Unit-III, IV and V.