BHARATHIDASAN UNIVERSITY, TIRUCHIRAPPALLI -620024.

M.Sc. Chemistry – Course Structure under CBCS

(applicable to the candidates admitted from the academic year 2008 – 2009 onwards)

Semester	Course	Course Title	Ins. Hrs/ Week	Credit	Exam Hrs	Marks		Total
						Int	Extn	
I	Core Course - I (CC)	Organic Chemistry I	6	5	3	25	75	100
	Core Course – II (CC)	Inorganic Chemistry I	6	5	3	25	75	100
	Core Course – III (CC)	Physical Chemistry I	6	5	3	25	75	100
	Core Course – IV (CC)	Organic Practical I	6	4	6*	40	60	100
	Core Course - V (CC)	Inorganic Practical I	6	4	6*	40	60	100
		Total	**30**	**23**				**500**
II	Core Course – VI (CC)	Inorganic Chemistry II	6	5	3	25	75	100
	Core Course -VII (CC)	Physical Methods in Chemistry I	6	5	3	25	75	100
	Core Course - VIII(CC)	Organic Practical II	6	4	6*	40	60	100
	Core Course -IX (CC)	Inorganic Practical II	6	4	6*	40	60	100
	Elective – I	Medicinal Chemistry / Bio organic Chemistry	6	4	3	25	75	100
		Total	**30**	**22**				**500**
III	Core Course -X (CC)	Organic Chemistry II	6	5	3	25	75	100
	Core Course – XI (CC)	Physical Methods in Chemistry II	6	5	3	25	75	100
	Core Course -XII (CC)	Physical Chemistry Practical I	6	4	6*	40	60	100
	Elective – II	Solid State Chemistry / Supramolecular Chemistry & Crystal Engineering	6	4	3	25	75	100
	Elective - III	Electro organic Chemistry / Analytical Chemistry	6	4	3	25	75	100
		Total	**30**	**22**				**500**
IV	Core Course -XIII (CC)	Physical Chemistry II	6	5	3	25	75	100
	Core Course –XIV(CC)	Physical Chemistry Practical II	6	4	6*	40	60	100
	Project Work	Dissertation=80 Marks [2 reviews –20+20=40 marks Report Valuation = 40 marks] Viva = 20 Marks	6	6	-	-	-	100
	Elective - IV	Green Chemistry / Industrial Chemistry	6	4	3	25	75	100
	Elective - V	Chemistry of Nanoscience & Nanotechnology	6	4	3	25	75	100
		Total	**30**	**23**				**500**
		Grand Total	**120**	**90**				**2000**

* Practical examination for Organic Chemistry Practicals I & II and Inorganic Chemistry Practicals I & II will be conducted at the end of second semester.

Practical examination for Physical Chemistry Practicals I & II will be conducted at the end of fourth semester

CORE COURSE I - ORGANIC CHEMISTRY I

UNIT – I

1. Structure and Bonding

Nomenclature of alicyclic, bicyclic and tricyclic compounds. (Basic skeletal structures only with or without one substituent)

Localized Chemical Bonding: Electronic Structure of molecules; VB, MO and HOMO-LUMO theory, Electronegativity, Dipole Moment, Inductive and Field Effects, Bond distances, Bond angles, Bond energies.

Delocalized Chemical Bonding: Bond energies and Bond distances in compounds containing delocalized Bonds, Cross conjucation, Resonance, Steric inhibition of resonance, Hyperconjugation, Keto – Enol Tautomerism.

2. Acids and Bases

Bronsted theory – Lewis acids and bases – Effect of structure on the strengths of acids and bases.

UNIT – II

3. Aromaticity

Aromatic character: six-, Five-, seven-, and eight-membered rings - Other systems with aromatic sextets – Huckel's theory of aromaticity, Concept of homoaromaticity and antiaromaticity, Electron occupancy in MO's and aromaticity - NMR concept of aromaticity and antiaromaticity, systems with 2,4,8 and 10 electrons, systems of more than 10 electrons, alternant and non-alternant hydrocarbons (azulene type). Bonding properties of systems with $(4n + 2)\pi$ electrons and $4n\pi$ electrons, Heteraromatic molecules. Annulenes and sydnones and fullerenes.

4. Heterocycles

Nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Synthesis, reactivity and applications of the following heterocycles: Pyrazoles, Oxazoles, Pyridazines, Pyrimidine and Pyrazines.

UNIT- III

5. Stereochemistry

Fundamentals of Organic Stereochemistry: Principles of symmetry – Stereoisomerism – Optical isomerism - Definitions – Conventions used in stereochemistry: Newman, Sawhorse and Fischer notations and interconversions and representations. Nomenclature, correlation of configuration. Cahn – Ingold – Prelog rules for simple molecules. Optical activity and chirality – Types of molecules exhibiting

optical activity – Fischer projection – Absolute configuration. Molecules with more than one chiral centre – Molecular chirality – Atropisomerism – Biphenyls, allenes and spiranes. Methods of determining configuration. Enantiomerism of compounds containing chiral heteroatoms – Walden inversion – Asymmetric synthesis based on Cram's rule – Enantiotopic behaviour and Prochiral centres.

6. Geometrical Isomerism

E & Z Nomenclature, Determination of configuration of geometrical isomers, Stereochemistry of addition and elimination reactions. Stereospecific and stereoselective synthesis – [Elementary examples].

7. Conformational Analysis

Basic concepts of conformational analysis – Conformations of *n*-butane, cyclohexane and decalins.

UNIT IV

8. Organic Photochemistry

Organic Photochemistry – Fundamental concepts – Jablonski diagram – Energy transfer, characteristics of photoreactions, photoreduction and photoxidation, photoreactions of ketones and enones, Norrish Type I and II reactions. Photochemistry of alkenes, dienes and aromatic compounds, reactions of unactivated centres – Photolytic cycloadditions and photolytic rearrangements – Photosenstitisation – Photoadditions – Barton reaction – Parterno Buchi reaction.

UNIT V

9. Reactive Intermediates

Carbocations, Carbanions, Carbenes and Nitrenes – Generation and stability of reactive intermediates. Correlation of reactivity with structure of reactive intermediates. Free radicals – Configurations – Identification by chemical and spectral methods – Free radical halogenation - NBS.

10. Methods of Determining Reaction Mechanisms

Types of reactions: Homolytic and Heterolytic cleavages of bonds, Characteristics of nucleophilic, electrophilic and free radical reactions. Thermodynamic and kinetic aspects, Hammond's postulate, isotope effects. Energy profile diagrams – Intermediate versus transition state, Product analysis and its importance, Crossover experiments, Kinetic methods, Stereochemical studies, Isotopic and substitutent effects.

References

1. J. March, Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 5th ed.,Wiley, 2000.
2. D. Nasipuri, Stereochemistry of organic compounds-Principles and applications, New Age International, 2nd Edition,2002.

3. I.L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS 1975.
4. R.K. Bansal, Organic Reaction Mechanisms, Tata McGraw Hill, 1975.
5. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th ed., Pearson, 1992.
6. J.D. Coyle, Organic Photochemistry - Wiley, 1985.
7. J.M. Coxon, B. Halton, Organic Photochemistry, Camb. Uni. Press, 2nd edition, 1987.
8. G.R. Chatwal , OrganicPhtochemistry, Himalaya Publications house, 1st edition, 1998.
9. P.S. Kalsi, Stereochemistry , Wiley eastern limited, New Delhi, 1990.

CORE COURSE II - INORGANIC CHEMISTRY I

UNIT – I

1. Main Group Chemistry

Chemistry of boron – borane, higher boranes, carboranes, borazines and boron nitrides. Chemistry of silicon – silanes, higher silanes, multiple bonded systems, disilanes, silicon nitrides, siloxanes and silicates. P-N compounds, cyclophosphazenes and cyclophosphazanes. S-N compounds – S_4N_4, $(SN)_x$.

2. Ionic Model

Lattice energy – Born-Lande equation - Kapustinski equation - High T_c superconductors – Solid state reactions – Types and examples.

UNIT II

3. Coordination Chemistry: Principles

Studies of coordination compounds in solution – detection of complex formation in solution – Stability constants – stepwise and over-all formation constants – simple methods (Potentiometric, pH metric and photometric methods) of determining the formation constants - Factors affecting stability – statistical and chelate effects – Forced configurations.

UNIT III

4. Theories of Metal - Ligand bond

VB theory and its limitations – Crystal field theory - splitting of d-orbitals under various geometries – Factors affecting splitting – CFSE and evidences for CFSE (Structural and thermodynamic effects) – Spectrochemical series – Jahn-Teller distortion – Spectral and magnetic properties of complexes – Site preferences - Limitations of CFT – Ligand field theory – MO theory – sigma – and pi-bonding in complexes – Nephelauxetic effect – The angular overlap model.

UNIT – IV

5. Coordination Chemistry – Reaction Mechanism

Kinetics and mechanism of reactions in solution – labile and inert complexes – Ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions – trans effect – theory and applications. Electron transfer reactions – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes – Application of Electron transfer reactions in inorganic - isomerisation and racemisation reactions of complexes – Molecular rearrangement – Reactions of four and six-coordinate complexes – Interconversion between stereoisomers. Reactions of coordinated ligands – Template effect and its application for the synthesis of Macrocyclic ligands – Unique properties.

UNIT - V

6. Inorganic Photochemistry

Electronic transitions in metal complexes, metal-centered and charge-transfer transitions – Various photophysical and photochemical processes of coordination compounds – Unimolecular charge-transfer photochemistry of cobalt(III) complexes. Mechanism of CTTM photoreduction. Ligand-field photochemistry of chromium(III) complexes, Adamson's rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium-polypyridine complexes, emission and redox properties – photochemistry of organometallic compounds, metal carbonyl compounds, compounds with metal-metal bonding Reinecke's salt chemical actinometer.

References

1. M. C. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd. 2nd ed.,1985.
2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 4th ed., A Wiley - Interscience Publication, John –Wiley & Sons, USA.
3. J.E. Huheey, Inorganic Chemistry 3rd. ed., Harper & Row publisher, Singapore.
4. A.W.Adamson, Inorganic Photochemistry, John Wiley & Sons, New York.
5. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, 1996.
6. A. W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, New York, 1975.
7. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley, New York, 1988.
8. F.Basolo and R.G.Pearson, Mechanism of Inorganic Reactions, John Wiley, New York.

CORE COURSE III - PHYSICAL CHEMISTRY I

UNIT – I

1. Group theory - Concepts

Elements of group theory – definition – group multiplication tables – conjugate classes, conjugate and normal subgroups – symmetry elements and operations – point groups – assignment of point groups to molecules, - Matrix representation of geometric transformation and point groups – reducible and irreducible representations– properties of irreducible representation – construction of character tables – bases for irreducible representation – direct product – symmetry adapted linear combinations – projection operators.

UNIT - II

2. Quantum Chemistry – I

Inadequacy of classical mechanics, Black body radiation, Planck's quantum concept, Photoelectric effect. Bohr's theory of hydrogen atom :Hydrogen spectra, Wave-particle dualism, Uncertainty principle, Inadequacy of old quantum theory.

Schrödinger equation, Postulatory basis of quantum mechanics. Operator algebra: operator, linear and hermitian, eigen functions and eigen values, angular momentum operator, commutation relations, related theorems.

Applications of wave mechanics to simple systems – particle in a box, one and three-dimensional, distortion of the box and Jahn-Teller effect, quantum numbers, zero-point energy, orthogonalisation and normality, finite potential barrier – tunneling.

UNIT – III

3. Chemical Kinetics- I

Theories of reaction rate – Absolute reaction rate theory (ARRT) - Significance of reaction co-ordinate – Potential energy surfaces – Kinetic isotope effect – Molecular dynamics – Marcus theory of electron transfer processes.

Principle of microscopic reversibility - Steady–state approximation – Chain reactions: thermal and photochemical reactions between hydrogen and halogens - Explosions and hydrogen – oxygen reactions.

UNIT – IV

4. Molecular Thermodynamics - I

Calculation of Thermodynamic probability of a system – Difference between thermodynamic probability and statistical probability – Ergodic hypothesis –Derivation of Boltzman distribution equation – physical significance of partition function- translational, rotational, vibrational and electronic partition functions – Quantum statistics – Bose – Einstein and Fermi – Dirac distribution equations – comparison of B.E and F.D statistics with Boltzman statistics – Concept of Negative Kelvin Temperature.

Relationships between partition function and thermodynamic properties such as E, H, Cp, Cv, P. Derivation of PV=RT, Molecular interpretation of entropy- Derivation of S=klnW- Establishment of analogous nature of S= klnW to ds= dq_{rev}/T. Calculation of S, A, G etc., from partition functions– calculation of equilibrium constants for very simple reactions.

UNIT – V

Fast reaction techniques: Introduction, flow methods (continuous and stopped flow methods)- Relaxation methods (T and P jump methods) – Pulse techniques (pulse radiolysis, flash photolysis, Shock tube method)- molecular beam method – lifetime method.

Photochemistry and Radiation Chemistry:

Photophysical processes electronically excited molecules Jablonski diagram – Stern-Volmer equation and its applications – experimental techniques in photochemistry – chemical actinometers –lasers and their applications.

Radiation Chemistry

Differences between radiation chemistry and photochemistry – sources of high energy radiation and interaction with matter – radiolysis of water, solvated electrons – Definition of G value – Curie –Linear energy transfer LET and Rad – Scavenging techniques- use of dosimetry and dosimeters in radiation chemistry- application of radiation chemistry.

References:

1. F. Albert Cotton, Chemical Applications of Group Theory, Third Edition John Wiley & Sons, Singapore 2003
2. Robert L. Carter, Molecular Symmetry and Group Theory John Wiley and Sons, Inc., New York, 1998.
3. R.L. Flurry, Jr, Symmetry Groups – Prentice Hall, New Jersy 1980.
4. B.E. Douglas and C.A. Hollingsworth, Symmetry in Bonding and Spectra – An Introduction, Academic Press,New York, 1985.
5. S.F.A. Kettle, Symmetry and Structure, John Wiley & Sons, Chichester, 1985.
6. A.K. Chandra, Introductory Quantum Chemistry, 4th ed,. Tata McGraw Hill 1994.
7. Doggett & Sutelife, Mathematics for chemists, Longman Scientific & Technical, New York, USA ,1995.
8. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1998.
9. F.L. Pillar Elementary Quantum Chemistry, McGraw Hill, 1968.
10. J.P. Lowe, Quantum Chemistry, Academic Press, 1978.
11. I.N. Levine, Quantum Chemistry, 5th edn, Prentice Hall, 2000.
12. P.W. Atkins, Molecular Quantum mechanics, Clarendon Press New York, 1973.
13. J. Goodisman, Contemporary Quantum Chemistry, Planum Press, New York, 1977.
14. R.K. Prasad, Quantum Chemistry, New Age International Publishers, New Delhi, 1997.
15. Horia Metiu, Quantum Mechanics, Taylor & Francis, New York, 2006.
16. Horia Metiu, Physical Chemistry, Kinetics Taylor & Francis, New York, 2006.

17. K.J. Laidler, Chemical Kinetics, 2nd ed., Tata McGraw Hill, 1975.
18. A.A. Frost and R.G.Pearson, Kinetics and Mechanism, John Wiley & Sons, New York, 1953.
19. D. A. Mc Quarrie and J. D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt Ltd, New Delhi, 2003.
20. J. N. Gurtu & A. Gurthu, Advanced Physical Chemistry, Pragathi Prakashan, Meerut , 2006.
21. R. Stephen Berry, Stuart A. Rice and John Ross, Physical Chemistry 2nd edn, Oxford Univ. Press, New York, 2000
22. J.I. Steinfeld, J.S.Francisco and W.L. Hase, Chemical Kinetics and Dynamics, 2nd edn, Prentice Hall,New Jersey, 1999.
23. K.S. Gupta, Chemical Kinetics & Reaction Mechanism , RBSA Publishers, Jaipur, India,1992.
24. R.K. Dave, Chemical Kinetics , Campus Books, 2000.
25. P.W. Atkins,Physical Chemistry, 7th edn, Oxford University press, 2002.
26. D. A. Mc Quarrie and D. Simon, Physical chemistry, A Molecular Approach ,Viva Books Pvt. Ltd, New Delhi, 2003.
27. J. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, Shobhan Lal Nagin, New Delhi, 1981.
28. D. A. Mc Quarrie, J. D. Simon, Molecular Thermodynamics, University Science Books, Sausalito, California, 1999.
29. F.W. Sears, Thermodynamics, Kinetic theory of Gases and Statistical Mechanics, 2nd Ed., Addition Wesley, 1972.
30. Horia Metiu, Physical Chemistry, Thermodynamics Taylor & Francis, 2006.
31. R.P.Wayne, Photochemistry, Butterworths,London(1970).
32. K.K.Rohatgi-Mukerjee, Fundamentals of Photochemistry , Wiley Eastern Ltd.,(1986)
33. G.Hughes, Radiation Chemistry, Oxford University Press (1973)
34. J.W.T Spinks and R.J. Woods, Introduction to Radiation Chemistry , 2nd ed., John Wiley & Sons (1976).

CORE COURSE IV - Inorganic Chemistry Practical – 1

Semi-micro qualitative analysis of a mixture containing two common and two rare cations.

Estimation of Copper, Ferric, Nickel, Chromium and Manganese using photoelectric colorimeter

CORE COURSE V - Organic Chemistry Practical -1

Qualitative Analysis of an organic mixture containing two components.

Pilot separation , bulk separation , analysis , derivatization.

Preparation of Organic compounds.(Single stage).

(a) methyl –m- nitrobenzoate from methylbenzoate (nitration)
(b) glucose pentaacetate from glucose (acetylation)
(c) resorcetophenone from resorcinol (acetylation)
(d) benzophenone oxime from benzophenone (addition)
(e) o-chlorobenzoic acid from anthranillic acid (Sandmayer reaction)
(f) P-benzoquinone from hydroquinone (oxidation)
(g) Phenyl-azo-2-napthol from aniline (diazotization)

SEMESTER II

CORE COURSE VI - INORGANIC CHEMISTRY II

BIOINORGANIC AND ORGANOMETALLIC CHEMISTRY

UNIT – I

General Principles of Bioinorganic Chemistry

Occurrence and availability of Inorganic elements in biological systems.

Biomineralisation

Control and assembly of advanced materials in Biology - Nucleation and crystal growth – various biominerals – calcium phosphate – calcium carbonate – Amorphous silica, Iron biominerals – strontium and barium sulphate.

Function and Transport of Alkali and Alkaline Earth Metal Ions

Characterization of K^+, Na^+, Ca^{2+} and Mg^{2+} - complexes of alkali and alkaline earth metal ions with macrocycles - Ion channels – ion pumps. Catalysis and regulation of bioenergetic processes by the Alkaline Earth Metal ions Mg^{2+} and Ca^{2+}.

Metals at the Center of Photosynthesis

Primary Processes in Photosynthesis – Photosystems I and II - Light Absorption (Energy Acquisition) – Exciton transport (Direct Energy Transfer) – Charge separation and electron transport – Manganese catalyzed oxidation of water to O_2.

UNIT – II

Cobalamines

Reactions of the alkyl cobalamins – One-electron Reduction and Oxidation – Co-C Bond Cleavage – coenzyme B_{12} – Alkylation reactions of methylcobalamin.

Heme and Non-heme Proteins

Hemoglobin and Myoglobin – Oxygen transport and storage – Electron transfer and Oxygen activation.Cytochromes, Ferredoxins and Rubredoxins – Model systems, mononuclear non-heme iron enzymes.

Copper Containing Proteins

Classification and examples - Electron transfer – Oxygen transport - Oxygenation – oxidases and reductases – Cytochrome c oxidase – Superoxide dismutase (Cu, Zn).

Nickel containing Enzyme: Urease.

UNIT – III

Medicinal Bioinorganic Chemistry

Bioinorganic Chemistry of quint essentially toxic metals. Lead, Cadmium, Mercury, Aluminium, Chromium, Iron, Copper, Plutonium. Detoxification by metal chelation. Drugs that act by binding at the metal sites of Metalloenzymes.

Chemotherapy

Chemotherapy with compounds of certain non-essential elements. Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action - Lithium in Pschycopharmocological drugs. Radiopharmaceuticals – Technetium.

UNIT IV

Hapticity, Ligand classification, synthesis and structure – The 18 electron rule – application and limitation- isolobal concept and its usefulness. Uses of typical organomettallics in organic synthesis such as metal alloys and organomettallic hydrides.Structure and bonding in metal carbonyls (simple and polynuclear) nitrosyl complexes – bridging and terminal nitrosyls, bent and linear nitrosyls. Dinitrogen complexes. Metallocene and arene complexes.Metal carbenes , carbynes, carboxylate anions.

UNIT – V

Reactions and Catalysis by Organomatallics

Organometallic reactions – Ligand association and dissociation – oxidative addition and reductive elimination – Insertion reactions – Reactions of coordinated ligands in organometallics - Hydrogenation, hydroformylation, epoxidation, metathesis, polymerization of olefins, olefin oxidation (Wacker process) and carbonylation of methanol.

Text Books and Reference Books

1. J. E. Huheey, Inorganic Chemistry, 3rd ed., Harper & Row Publishers, Singapore.
2. Purcell and Kotz, Inorganic Chemistry, Saunders Golden Sunburst Series, W. B. Saunders Company, Philadelphia.
3. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry , Panima Publishing Company, New Delhi, 1997.
4. W. Kaim and B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life , John Wiley & Sons, New York, USA.
5. Cotton and Wilkinson, Advanced Inorganic Chemistry, 5th ed., Wiley Interscience Publication, John Wiley & Sons, New York, USA.
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7. G. L. Eichorn, Inorganic Biochemistry, Volumes 1 & 2, 2nd ed., Elsevier Scientific Publishing Company, New York, 1973.
8. F. A. Cotton and G. Wilkinson, Inorganic Chemistry, John Wiley & Sons, New York.
9. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley & Sons, New York.
10. S. E. Kegley and A. R. Pinhas, Problems and Solutions in Organometallic Chemistry, University Science Books, Oxford University Press.
11. A. J. Pearson, Metalloorganic Chemistry,
12. A. W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry
13. I. Haiduc and J. J. Zuckerman, Basic Organometallic Chemistry
14. P. Powell, Principles of Organometallic Chemistry, 2nd ed., Chapman and Hall, London.
15. B. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry, 2nd ed, John Wiley & sons, New York.
16. Oxford Chemistry Primers Series, No. 12, M. Bochmann Organometallics 1: Complexes with transition metal-carbon σ bonds and No. 13 M. Bochmann Organometallics 2: Complexes with transition metal-carbon π-bonds
17. J. P. Collman, L. S. Hegedus, J. R. Nortan and R. G. Finke, Principles and Applications of Organotransition Metal Chemistry, University Science Books. Mill Valley, California.
18. R. Hoffmann, Angew. Chem. Int. Ed., Engl. 21, 711-800 1982.

CORE COURSE VII - PHYSICAL METHODS IN CHEMISTRY - I

UNIT I

Theoretical principles of Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecular systems – Time evolution of the systems under radiation – Einstein transition probability for induced absorption and spontaneous and stimulated emission – Transition moment and Oscillator strength

Microwave spectroscopy – rotational spectra of diatomic molecules, rigid and nonrigid rotors, - Intensity of spectral lines, - Effects of isotopic substitution – Microwave spectra of polyatomic molecules – Linear and symmetric top molecules, Infrared spectra – diatomic molecules, simple harmonic and anharmonic oscillators, - diatomic vibrating rotator, rotation-vibration spectrum of carbon monoxide, - Interaction of rotation and vibration (breakdown of Born – Oppenheimer approximation) – Influence of the rotation on the spectrum of polyatomic molecules, linear and symmetric top molecules, parallel and perpendicular vibrations, Influence of nuclear spin.

Raman spectra – Rotational Raman spectra of linear and symmetric top molecules – Vibrational Raman spectra, Rotational fine structure. Electronic spectra of diatomic molecules, - Vibrational coarse structure – Intensity of vibrational lines in electronic spectra – Rotational fine structure – Fortrat digram.

UNIT II

Advanced Spectroscopy : **NMR**

^{1}H NMR Spectroscopy – Multiplicity – Coupling constant – First order and second order proton, Spin - spin splitting – Dependence of J on dihedral angle – Vicinal and geminal coupling constants – Karplus equation – long range coupling constants, Influence of stereochemical factors on chemical shift of protons. Simplification of complex spectra – Double resonance techniques, shifts reagents. Chemical spin decoupling of rapidly exchangable protons (OH, SH, COOCH, NH, NH_2), an elementary treatment of NOE phenomenon. ^{13}C NMR Spectroscopy – Basic theory of FT – NMR, Relaxation – Broad band decoupling. Off resonance decoupling and chemical shifts of common functional groups, DEPT spectra. Identification of small compounds based on NMR data. 2D Techniques: ^{1}H – ^{1}H COSY, ^{1}H – ^{13}C COSY – HMBC and NOESY.

UNIT III

Advanced Spectroscopy: UV –Vis, IR

UV-Visible Spectroscopy : Introduction - Instrumentation, Sampling techniques - Woodward–Fieser and Scott rules for conjucated dienes and polymers, ketones, aldehydes, α,β-unsaturated acids, esters, nitriles, and amides. Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives - Study of steric effect in aromaticity.

Infrared Spectroscopy : Introduction - Instrumentation, Sampling techniques, factors influencing group frequencies – Both internal and external – quantitative studies. Hydrogen bonding – (intermolecular and intramolecular).

UNIT IV

Electron spin resonance spectroscopy: Basic principles – comparison between esr and nmr spectra – hyperfine splitting – factors affecting the magnitude of g – values – calculation of unpaired electron density on an atom in a delocalized system – applications to organic free radicals.

Optical rotatory dispersion and circular dichroism : Introduction to theory and terminology – cotton effect – ORD curves – axial haloketone rule and its applications – octant rule – its applications – applications of ORD to determine absolute configuration of monocyclic ketones – comparision between ORD and CD – their inter relationships.

Mass Spectrometry

Instrumentation – Resolution, EI and CI methods – Base peak, isotopic peaks, metastable peak, parent peak, determination and use of molecular formula, recognition of molecular ion peak – FAB. Fragmentation – General rules – Pattern of fragmentation for various classes of compounds, McLafferty rearrangement, Importance of metastable peaks.

UNIT V

X-ray diffraction: X-ray diffraction by single crystal – Space groups –Systematic absences in X-ray data and identification of lattice types , glide planes and screw axes.X-ray intensities, structure factor and its relation to intensity and electron density , phase problem. Structure solution by Heavy atom method and direct method. Determination of absolute configuration of molecules. A brief account of Cambridge Structural Database (CSD) and Protein Data Bank (PDB).

Electron Diffraction by gases - Scattering intensity vs Scattering angle, wierl equation, measurement technique, elucidation of structure of simple gas phase molecules.

Neutron diffraction by crystals – magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

References:

1. C.N. Banwell, Fundamentals of molecular Spectroscopy, 3rd ed., TMH, New Delhi, 1983.
2. B.P. Straughan and S.Walker Spectroscopy Vol.3, Chapman Hall London, 1976.
3. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1964.
4. P.K.Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley New York, 1989.
6. P.M. Silverstein, F. X. Wester, Spectroscopic Identification of Organic Compounds, 6th ed., Wiley 1998.
7. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
8. J.R. Dyer, Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall, 1965.
9. Y.R. Sharma , Elementary Organic Spectroscopy – Principles and Chemical applications, S.Chand,1992.
10. P.S.Kalsi, Spectroscopy of Organic Compounds.
11. Clegg,W., Crystal structure determination, Oxford University press , New York,1998.

12.Stout,G.H., Jensen , L.H. X-ray structure determination : A practical guide , John wiley & sons Publication: New York,1989

13.Glusker, J.P., Trueblood,K.N. Crystal structure analysis: A primer., Oxford university press, New York, 1972.

Webpages :

Cambridge Structural Database (CSD) - http://www.ccdc.cam.ac.uk/products/csd/

Protein Data Bank (PDB) - http://www.rcsb.org/pdb/home/home.do

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CORE COURSE VIII - ORGANIC CHEMISTRY PRACTICAL-II

Quantitative analysis of organic compounds

Estimation of phenol, aniline, ketone, glucose, nitrobenzene, saponification value of an oil and Iodine value of an oil.

Preparation of organic compounds (Double stage)

a. p-bromo acetanilide from aniline (acetylation and bromination).
b. acetyl salicylic acid from methyl salicylate (hydrolysis and acetylation).
c. 1,3,5-tribromobenzene from aniline (bromination, diazotization and hydrolysation).
d. p-nitroaniline from acetanilide (nitration and hydrolysis).
e. benzillic acid from benzoin (rearrangement).
f. p-amino benzoic acid from p-nitro toluene (oxidation and reduction).
g. benzanilide from benzophenone (rearrangement).
h. p-bromoaniline from acetanilide (bromination and hydrolysis).
i. m-nitroaniline from nitrobenzene (nitration and reduction).
j. 1,2,4-triacetoxy benzene from hydroquinone (oxidation and acylation).

CORE COURSE IX - INORGANIC CHEMISTRY PRACTICAL-II

Titrimetry and Gravimetry

A mixture of solution(s) should be given for estimation

Cu (V) and Ni (G)
Cu (V) and Zn (G)
Fe (V) and Zn (G)
Fe (V) and Ni (G)
Zn (C) and Cu (G)

Preparation of the following compounds

a. Tetramminecopper (II) sulphate.
b. Potassium trioxalatochromate (III).
c. Potassium trioxalatoaluminate (III).
d. Trithioureacopper (I) chloride.
e. Trithioureacopper (I) sulphate.
f. Dibenzyltin dichloride.

ELECTIVE I (Medicinal Chemistry / Bio organic chemistry)

MEDICINAL CHEMISTRY

UNIT-I: Introduction to Drugs and Their Action

Drugs: Historical background-sources and classification of drugs-important terminologies in medicinal chemistry. Drug Action: role of intermolecular forces-drug targets: lipids, carbohydrates, proteins (enzymes, receptor) and nucleic acids as drug targets. Pharmacokinetics and pharmacodynamics: administration, absorption, distribution, metabolism, elimination of drugs-bioavailability of drugs-side effects.

UNIT-II: Selected Examples of Drugs and Their Mechanism of Action

Antibacterial agents-mechanism of action-antibacterial agents that act against cell metabolism (sulfonamides), inhibit cell wall synthesis (penicillins, cephalosporins), interact with plasma membrane (valinomycin and gramicidin A), impair protein synthesis (tetracyclines, chloramphenicol) and act on nucleic acids (quinolones and fluoroquinolones, rifamycins). Antiviral agents-general principles-nucleic acid synthesis inhibitors (HIV), host cell penetration inhibitors, inhibitors of viral protein synthesis. Antifungal agents-azoles, allyamines and phenols. Anticancer drugs and their mechanism of action- role of antimetabolites, antisense drugs, alkylating agents and interchelating agents in cancer chemotherapy. Cardiovascular drugs: antiarrhythemic and antihypertension drugs.

UNIT-III: Drug Discovery, Design and Development

Identification of diseases and corresponding targets, bioassays and leads. Stereochemistry and solubility issues in drug design. Structure activity relationships (SARs): changing size and shape-introduction of new substituents. Quantitative structure activity relationships (QSARs): lipophilicity-electronic and steric effects-Hansch Analysis-Topliss decision tree. Chemical and process development of drugs. Preclinical trials: pharmacology, toxicology, metabolism and stability studies-formulation. Clinical trials: phase I-IV studies-ethical issues. Patent protection. Regulation

UNIT-IV: Lead and Analogue Synthesis-1

Designing organic synthesis-disconnection approach-synthons and synthetic equivalents-one group disconnections: alcohol, olefin, ketone, acids-two group disconnections:1,2-, 1,3-, 1,4- and 1,5-difunctional compounds-convergent synthesis-functional group interconversions- functional group additions-carbon-heteroatom bonds-methods for 3- to 6-membered rings.

UNIT-V: Lead and Analogue Synthesis-2

Combinatorial synthesis in medicinal chemistry: Solid phase techniques-methods of parallel synthesis-mix and split techniques-dynamic combinatorial chemistry-screening and deconvolution-limitations of combinatorial synthesis

Assymmetric synthesis: basic principles-stereoselective and stereospecific reactions- methods for determining enantiomeric excess-chiral auxiliary, reagents and catalysts and their applications (wherever applicable) in alkylation, hydrogenation, hydroxylation, epoxidation and hydroboration of alkenes, reduction of ketones-Cram and Felkin-ahn models. Noyori's BINAP – Jacobson catalyst – Evans catalyst.

References:

1) Fundamentals of Medicinal Chemistry by Gareth Thomas, John Wiley & Sons: Chichester, **2003**.
2) Medicinal Chemistry: An Introduction by Gareth Thomas, Wiley-Interscience, 2nd edition, **2008**.
3) An introduction to Medicinal Chemistry by Graham L. Patric, Oxford University Press, USA, 3rd edition, **2005**.
4) Wilson and Giswald's Textbook of Organic Medicinal and Pharmaceutical Chemistry by John Block and John M Beale (Eds), Lippincott Williams & Wilkins, 11th edition, **2003**.
5) The Organic Chemistry of Drug Design and Drug Action by Richard B. Silverman, Academic press, 2nd edition, **2004**.
6) Designing Organic Synthesis: The Disconnection Approach by Stuart Warren, Wiley, 2nd edition, **1984**.
7) Asymmetric Synthesis by H. B. Kagan, Thieme Medical Publishers, **2003**.
8) Advanced Organic Chemistry: Part-A and Part-B by Francis A. Carey and Richard B. Sundberg, Springer, 5th edition, **2007**.

OR

BIOORGANIC CHEMISTRY

UNIT-1: Amino Acids and Proteins

Structure, classification, synthesis and properties of amino acids, isoelectric point, biosynthesis of amino acids. Peptides: oligo- and polypepides, geometry of peptide linkage, N-terminal and C-terminal residue analysis, synthesis of peptides-amino and carboxyl protecting groups-solid phase peptide synthesis. Proteins: classification and properties (denaturation, isolelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins, collagen and triple helix.

UNIT-2: Enzymes and Cofactors

Mechanism of enzyme catalysis, Factors influencing enzyme action, Examples of typical enzyme mechanisms: chymotrypsin, ribonuclease and lysozyme, Enzyme-catalyzed addition, elimination, condensation, carboxylation and decarboxylation, isomerisation, group transfer and rearrangement reactions-structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid and Vitamin B12. Mechanisms of reactions catalysed by the above cofactors.

UNIT-III: Nucleic Acids and Protein Synthesis

Nucleotides and nucleosides, DNA: primary and secondary structure-replication of DNA. RNA and protein synthesis: Messenger RNA synthesis-transcription, Ribosomes-rRNA, Transfer RNA, genetic code-translation. Determination of base sequence of DNA. Polymerase Chain Reaction (PCR). Antisense technology in chemotherapy and other nucleic acid-targeted drugs-intercalaters, sequence specific drugs. A brief account of ribosyme and iRNA.

UNIT-IV: Lead and Analogue Synthesis-1

Designing organic synthesis-disconnection approach-synthons and synthetic equivalents-one group disconnections: alcohol, olefin, ketone, acids-two group disconnections:1,2-, 1,3-, 1,4- and 1,5-difunctional compounds-convergent synthesis-functional group interconversions- functional group additions-carbon-heteroatom bonds-methods for 3- to 6-membered rings.

UNIT-V: Lead and Analogue Synthesis-2

Combinatorial synthesis in medicinal chemistry: Solid phase techniques-methods of parallel synthesis-mix and split techniques-dynamic combinatorial chemistry-screening and deconvolution-limitations of combinatorial synthesis

Assymmetric synthesis: basic principles-stereoselective and stereospecific reactions- methods for determining enantiomeric excess-chiral auxiliary, reagents and catalysts and their applications (wherever applicable) in alkylation, hydrogenation, hydroxylation, epoxidation and hydroboration of alkenes, reduction of ketones-Cram and Felkin-ahn models. Noyori's BINAP – Jacobson catalyst – Evans catalyst.

References:

1.Bioorganic Chemistry: A Chemical approach to Enzyme action, Hermann Dugas and C.Penny, Springer-Verlag.
2.Fundamentals of Enzymology,N.C. Price and L.Stevens, Oxford University Press.
3.Enzymatic Reaction Mechanisms, C. Walsh, W.H.Freeman.
4. Designing Organic Synthesis: The Disconnection Approach by Stuart Warren, Wiley, 2nd edition, 1984.
5.Asymmetric Synthesis by H. B. Kagan, Thieme Medical Publishers, 2003.
6.Advanced Organic Chemistry: Part-A and Part-B by Francis A. Carey and Richard B. Sundberg, Springer, 5th edition, 2007.

SEMESTER III

CORE COURSE X - ORGANIC CHEMISTRY II

UNIT – I

Nucleophilic Substitution Reactions

Aliphatic Nucleophilic substitution – Mechanisms – Effect of structure - Stereochemical factors – Neighbouring group participation, substitutions at allylic and vinylic carbons. Correlation of structure with reactivity – Solvent effects.Rearrangements involving Carbocations - Wagner Meerwein and Dienone – phenol rearrangements.

Aromatic Nucleophilic substitution – S_N1 S_NAr ,Benzyne mechanism – reactivity orientation – Ullman,Sandmeyer and Chichibabin reaction.Rearrangements involving nucleoplilic substitution – Stevens – sommelet Hauser and Von – Richter rearrangements.

UNIT - II

Electrophilic Substitution Reactions

Aromatic electrophilic substitution reaction - Orientation, reactivity and mechanisms based on transition state theory with suitable reactions, substitutions in Thiophene, Pyridine and Pyridine-N-Oxide. Quantitative treatment of the structural effects on reactivity. Substituents effects – Origins of Hammett equation – Principles of Hammett correlation – Effect of structure on reaction mechanisms Hammett parameters; σ and ρ, modified forms of Hammett equation. Taft Equation.

Aliphatic Electrophilic Substitution: SE^2,SE^i and SE^1mechanisms ,Diazonium coupling reactions. Metals as electrophile in substitution reactions and decomposition of diazonium salts.

UNIT – III

Addition and Elimination Reactions

Addition to carbon – carbon multiple bonds: Electrophilic, nucleophilic and free radical additions – Orientation of the addition – Stereochemical factors influencing the addition of bromine and hydrogen bromide, hydroxylation, hydroboration leading to formation of alcohols. Addition to carbonyl and conjugated carbonyl systems - Mechanism – Grignard reagents – 1,2 and 1,4-additions (dimethyllithiumcuprate),Benzoin , Knovenagel, Stobbe and Darzen's glycidic ester condensation and Reformatsky reactions.

Elimination Reactions: Mechanisms; E1,E2, E1cB – Stereochemistry of elimination, Hofmann and Saytzeff rules – Competition between elimination and substitution - Pyrolytic cis elimination, Chugaev reaction – Examples such as dehydration, dehydrohalogenatio, Hofmann degradation, Cope elimination – Bredt's rule with examples.

UNIT – IV

Pericyclic Reactions and Rearrangements

Concerted reactions – stereochemistry-orbital symmetry and concerted symmetry and correlation diagram –Frontier molecular orbital approach – Woodward and Hoffmann rules – Electrocylcic reactions – cycloaddition reactions – sigmatropic rearrangements – selection rules and examples with simple molecules – 1,3 and 1,5 hydrogen shifts –Cope and Claisen rearrangements. Other molecular rearrangements Wolff – Lossen – Schmidt – Favorski – Pummmerer and Hofman Freytas reagents

UNIT V

Reagents in Organic Synthesis

Reduction: Catalytic hydrogenation – Wilkinson Catalyst, dehydrogenation, reduction with LAH, $NaBH_4$, tertiarybutoxy aluminum hydride, $NaCNBH_3$, tributyltin hydride, alkali metals for reduction, reductions involving hydrazines,Wolf Kishner reduction.

Oxidation: Osmium tetroxide, Sharpless asymmetric epoxidation, Chromyl chloride, Ozone, DDQ, Dioxiranes, Lead tetraacetate, Selenium dioxide, DMSO with either Ac_2O or Oxalyl chloride, Dess-Martin reagent. Synthesis involving phase transfer catalysis (PTC),use of crown ethers, Merrifield resin, Baker's yeast

References

1. S.H. Pine, J.B. Hendrickson, D.J. Cram and G.S. Hammond, Organic chemistry, McGraw Hill, 4th ed., 1980.
2. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry,Harper and Row, 1976.
3. J. March, Advanced Organic Chemistry; Reactions, Mechanisms and Structure, 5th Ed., Willey, 2000.
4. R.K. Bansal, Reaction Mechanism in Organic Chemistry, Tata McGraw Hill, 1990.
5. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Parts A & B, Plenum, 2002.

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CORE COURSE XI - PHYSICAL METHODS IN CHEMISTRY – II

UNIT I

Electronic Spectroscopy

Microstates, terms and energy levels for d^1 – d^9 ions in cubic and square fields – Intensity of bands – group theoretical approach to selection rules - Effect of distortion and spin-orbit coupling on spectra – Evaluation of 10Dq and β for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of $[Ru(bipy)_3]^{2+}$.
Optical rotatory dispersion and circular dichroism and Magnetic circular dichroism – applications to metal complexes.

UNIT – II

Infrared and Raman Spectroscopy

Vibrations in simple molecules (H_2O, CO_2) and their symmetry notation for molecular vibrations – Group vibrations and the limitations- combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3 -, ClO^-_4 – effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate,

nitrate, sulphate and dimethyl sulfoxide – Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment) – Applications of Raman Spectroscopy – Resonance Raman Spectroscopy. Mass Spectrometry: Principles and presentation of spectra – molecular fragmentation – ion reactions – Inorganic applications.

UNIT – III

NMR Spectroscopy

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^{1}H, ^{19}F, ^{31}P, ^{13}C) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei (^{2}H, ^{10}B, ^{11}B) on the ^{1}H NMR spectra, Satellite spectra.

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Systems with chemical exchange - evaluation of thermodynamic parameters in simple systems – study of fluxional behavior of molecules – an elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents.

UNIT IV

EPR spectroscopy

Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

Magnetic properties:

Types of magnetism – Dia –para – ferro and antiferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Second order Zeeman effect – states KT – states<<KT. Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism. Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds.

UNIT V

Mossbauer Spectroscopy

Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – applications to iron and tin compounds.

NQR spectroscopy

Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

REFERENCES:

1. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern Company .
2. R.S.Drago, Physical Methods in Chemistry, W.B. Saunders Company, Philadelphia, London.
3. F.A. Cotton and G.Wilkinson, Advanced Inorganic Chemistry, 3rd ed., Wiley-Eastern Company, New Delhi 1990.
4. P.J. Wheatley, The Determination of Molecular Structure, .
5. Lewis and Wilkins, Modern Coordination Chemistry,.
6. E.A.V.Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, 1987.

CORE COURSE XII - PHYSICAL CHEMISTRY PRACTICAL-I

Any ten experiments (to be dedided by the course teacher) out of the following experiments.

a. Kinetics- Acid hydrolysis of ester- Comparison of strengths of acids.
b. Kinetics- acid hydrolysis of Ester- Determination of energy of activation (Ea).
c. Kinetics- Saponification of Ester- Determination of Ea by conductometry.
d. Kinetics- Persulphate- Iodine reaction- Determination of order, effective of ionic strength on rate constant.
e. Determination of molecular weight of substance by Transition Temperature method.
f. Determination of molecular weight of substances by Rast method.
g. Determination of Critical Solution Temperature (CST) of phenol- water system and effect of impurity on CST.
h. Study of phase diagram of two components forming a simple eutectic.
i. Study of phase diagram of two compounds forming a compound.
j. Study of phase diagram of three components system.
k. Determination of molecular weight of substances by cryoscopy.
l. Determination of integral and differential heat of solutions by colorimetry.
m. Polymerization- Rate of polymerization of acrylamide.
n. Distribution law- Study of Iodine- Iodine equilibrium.
o. Distribution law- Study of association of benzoic acid in benzene.
p. Adsorption- Oxalic acid/Acetic acid on charcoal using freundlich isotherm.

ELECTIVE PAPER II

(Solid State Chemistry / Supramolecular Chemistry & Crystal Engineering)

SOLID STATE CHEMISTRY

UNIT 1

Concepts and Languages of supramolecular chemistry. Various types of non-covalent interactions. Hydrogen bonds, C-H…X interactions, Halogen bonds. π – π interactions,non – bonded interactions. Various types of molecular recognition.

Crystal engineering of Organic solids: Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs. Concepts of different types of synthons based on non-covalent interactions. Principles of crystal engineering and non-covalent synthesis. Polymorphism and Pseudopolymorphism. Supramolecular isomorphism / polymorphism. Crystal engineering of pharmaceutical phases.

UNIT II

M.O.F (Metallo Organic Frame works), Organometallic systems. Combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. Design of nanoporous solids. Inter ligand hydrogen bonds in metal complexes – implications for drug design. Crystal engineering of NLO materials, OLED.

UNIT III

Preparative methods in solid state chemistry:

General principles of solid state chemistry - Experimental procedure, Coprecipitation as a precursor to solid state reaction, Other precursor methods, Kinetics of solid state reactions - Crystallizations of solutions, melts, glasses and gels,Solutions and gels : zeolite synthesis, Melts, Glasses - Vapour phase transport methods - Modification of existing structures by ion exchange and intercalation reactions,Graphite

intercalation compounds, Transition metal dichalcogenide and other intercalation compounds, Ion exchange reaction, Synthesis of new metastable phases by 'Chimie Douce' - Electrochemical reduction methods - Preparation of thin films,Chemical and electrochemical methods, Physical methods - Growth of single crystals,Czochralski method,Bridgman and stockbarger methods, Zone melting, Precipitation from solution or melt : flux method, Epitaxial growth of thin layers, Verneuil flame fusion method, Vapour phase transport , Hydrothermal methods, Comparison of different methods - High pressure and hydrothermal methods, Hydrothermal methods, Dry high pressure methods.

UNIT IV

Magnetic Materials:

Selected examples of magnetic materials, their structures and properties - Metals and alloys, Transition metal oxides, Spinels, Garnets, Ilmenites and perovskites, Magnetoplumbites - Applications: structure/property relations: Transformer, Information strorage, Magnetic bubble memory devices, Permanent magnets.

Optical Properties: Luminescence, Lasers : Luminescence and phosphors -Definitions and general comments, Configurational coordinate model, Some phosphor materials, Anti-Stokes phosphors – Lasers-The ruby laser,Neodymium lasers

UNIT V

Organic solid state chemistry:

Topochemical control of solid state organic reactions: Intramolecular reactions : conformational effects , Intermolecular reactions : moleculare packing effects,Photodimerization of o-ethoxy-trans-cinnamic acid (α form, β form, γ form),Photopolymerization of 2, 50distyrylpyrazine, Photopolumerizations of diacetylenes,Assymetric syntheses, Dimerization of anthracene – role of crystal defects, Control of molecular packing arrangements, Organic reactions within inorganic host structures - Electrically conduction organic solids : organic metals, Conjugated systems, Doped polyacetylene, Polyparaphinylene , Polypyrrole. - organic charge transfer complexes : new superconductors

References:

1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
2. Desiraju, G.R. Crystal Engineering: The Design of Organic Solids,Elsevier, Amsterdam, 1989.
3. Desiraju, G.R. & Steiner, T. The weak Hydrogen Bond in Structural Chemistry and Biology: Oxford University press: Oxford, 1999.
4. Jeffrey, G. A. Introduction to Hydrogen Bonding ; Oxford University press: New York, 1997.
5. Lehn, J.M. Transition metals in supramolecular chemistry : John Wiley & sons: New York, 1999.
6. Desiraju, G.R. (2001). Current Science, 81, 1038.
7. Rao, C.N.R. (2001). Current Science, 81, 1030.
8. Solid state chemistry and its applications by Anthony R.West, John Wiley & sons (For Unit III – V, Page no. (562-593,666-679))
9. "Molecule Matters" Saravanakumar, k & Sankararaman, S.,(2007).Resonance,Vol.12, No 11, Page 77.
9. Journals
   (i) Crystal Growth and Design. http://www.pubs.acs.org/journals/cgdefu/index.html
   (ii)Crystal Engineering Communication, http://www.rsc.org/Publishing/Journals/ce/index.asp

SUPRAMOLECULAR CHEMISTRY & CRYSTAL ENGINEERING

UNIT 1

Concepts and Languages of supramolecular chemistry. Various types of non-covalent interactions. Hydrogen bonds, C-H…X interactions, Halogen bonds. π – π interactions,non – bonded interactions. Various types of molecular recognition.

Crystal engineering of Organic solids: Hydrogen bonded supramolecular patterns involving water / carboxyl / halide motifs. Concepts of different types of synthons based on non-covalent interactions. Principles of crystal engineering and non-covalent synthesis. Polymorphism and Pseudopolymorphism. Supramolecular isomorphism / polymorphism. Crystal engineering of pharmaceutical phases.

UNIT II

M.O.F (Metallo Organic Frame works), Organometallic systems. Combinations of different interactions to design molecular rods, triangles, ladders, networks, etc. Design of nanoporous solids. Inter ligand hydrogen bonds in metal complexes – implications for drug design. Crystal engineering of NLO materials,OLED.

UNIT III

Corecptor Molecules and Multiple Recognition:
Dinuclear and Ploynulclear Metal ion Cryptates. Linear recognition of molecular length by Ditopic Coreceptors. Heterotopic Coreceptors- Cyclophane Receptors, Amphiphillic Receptors, Large molecular cages. Multiple Recognition in Metalloreceptors. Supramolecular dynamics.

UNIT IV

Supramolecular Reactivity and Catalysis
Catalysis by Reactive Macrocyclic Cation Receptor Molecules. Catalysis by Reactive Anion Receptor Molecules. Catalysis with Cyclophane Type Receptors.Supramolecular Metallocatalysis. Cocatalysis: Catalysis of Synthetic reactions. Biomolecular and Abiotic catalysis

Supramolecular Chemistry in solution: Cyclodextrin, Micelles, Dendrimmers, Gelators. Classification and typical reactions- Applications.

UNIT V

Supramolecular Devices and Sensors: Various types of supramolecular devices – an overview. Supramolecular Photochemistry: Molecular and Supramolecular Photonic Devices – Light conversion and Energy transfer Devices. Molecular and Supramolecular Electronic Devices – Electronic conducting Devices - Molecular wires, Modified and Switchable Molecular wires. Molecular and Supramolecular Ionic Devices – Tubular Mesophases, Molecular Protonics. Switching Devices: Photo switching and Electro switching. Ion and molecule sensors. Role of supramolecular chemistry in the development of nanoscience and technology.

References:

1. Lehn, J.M. Supramolecular Chemistry, VCH, Wienheim, 1995.
2. Desiraju, G.R. Crystal Engineering: The Design of Organic Solids, Elsevier, Amsterdam, 1989.
3. Desiraju, G.R. & Steiner, T. The weak Hydrogen Bond in Structural Chemistry and Biology: Oxford University press: Oxford, 1999.

4. Jeffrey, G. A. Introduction to Hydrogen Bonding ; Oxford University press: New York, 1997.

5. Lehn, J.M. Transition metals in supramolecular chemistry : John Wiley & sons: New York, 1999.

6. Desiraju, G.R. (2001). Current Science, 81, 1038.

7. Rao, C.N.R. (2001). Current Science, 81, 1030.

8. "Molecule Matters" Saravanakumar, k & Sankararaman, S,(2007).Resonance,Vol.12, No 11, Page 77.

9. Journals

(i)Crystal Growth and Design, http://www.pubs.acs.org/journals/cgdefu/index.html

(ii)Crystal Engineering Communication, http://www.rsc.org/Publishing/Journals/ce/index.asp

ELECTIVE III (Electro organic chemistry / Analytical Chemistry)

ELECTRO ORGANIC CHEMISTRY

UNIT I

Basic concepts of electro organic synthesis:

Introduction, fundamental aspects of electro transfer reaction : oxidation, reduction reactions vs electron transfer reactions in organic chemistry and electrochemistry - Standard potentials : Mechanism and theory of outer sphere electron transfer reactions – Fundamental aspects of electrode phenomena, monitoring a half-reactions, general view of an electrode reaction, adsorption phenomena – Mass transfer in electro chemistry, fundamental aspects, steady state electrochemical methods, Transient electrochemical methods.

UNIT II

Methods for studies of electrochemical reactions :

Introduction, linears sweep voltammetry and cyclic voltammetry, Experimental setup, simple electrotransfer reaction, electron transfer reaction followed by chemical reaction and solutions, limiting experimental factors – potential step and current step method, chronoamperometry, chronocoulometry, chronopotentiometry – polarography – methods for determination of number of electrons.

UNIT III

Cathodic reductions :

Introduction, formation of radical anions, dianions and polyanions, experimental aspects, thermodynamics kinetics, addition of electrophilic reagents and related reaction, dimerization.

Electrochemical reduction of halogenated compounds : monohalogenated alkanes, halogenated aromatic compounds, acyl halides, aliphatic alpha – halo carbonyl compounds, cathodic reduction of nitro and related compounds, Aliphatic nitro compounds, aromatic nitro compounds(preparation of para amino phenol nitrobenzenes, nitramines and azides). Eletrochemical reduction of carbonyl compounds, general aspects.

UNIT IV

Anodic oxidation of organic compounds:

Introduction, general mechanistic consideration, direct anodic oxidation, indirect anodic oxidation. Anodic oxidation of hydrocarbons, nitrogen containing compounds.

Electrosynthesis of Bioactive materials:
Introduction, simple Kolbe oxidation: application to synthesis of (+) - α onxerin and (+) - penta cyclosqualene, Kolbe cyclisation and Tandem cyclization.

UNIT V

Special topic in electro organic synthesis:

Paired electro organic synthesis, simple examples – electrogenerated reagents Homogeneous redox catalysts – General aspects of indirect electron exchanges, pure redox catalysis (general case) – use of indirect electrochemical reactions in sythesis, oxidations, reductions – Electrogenarated superoxides.

Electrochemical partial fluorination : Introduction, Anodic fluorination of aromatic compounds, olefins, carbonyl compounds, heterocyclic compounds.

Electro enzymatics synthesis : Introduction, principles of redox catalytic enzyme activation and co-factor regeneration – electroenzymatic reductions and oxidation (simple examples only).

Reference:

Organic electro chemistry by Henning Lund & Ole Hammerich, , 4th edition,
Publisher: Marcel Dekker, Inc, New York.

OR

ANALYTICAL CHEMISTRY:

UNIT 1

Instrumental methods of Analysis:

Principles and Applications of Extended X-ray absorption fine structure (EXAFS) – Surface extended X-ray absorption (SEXAFS) – Atomic Absorption Spectroscopy (AAS) - Flame Emission Spectroscopy (FES) . Turbidimetry – Theory and Applications.

UNIT II

Data and Error Analysis :

Various types of Error – Accuracy, precision, significant figures – Frequency distributions, the binomial distribution, the Poisson distribution and normal distribution – Describing data, population and sample, mean, variance, standard deviation, way of quoting uncertainty, robust estimators, repeatability and reproducibility of measurements – Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t-Test, Paired t-Test – Analysis of variance (ANOVA) – Correlation and Regression – Curve fitting , Fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – General polynomial equation fitting , linearizing transformations, exponential function fit – r and its abuse – multiple linear regression analysis, elementary aspects.

UNIT III

Chromatography:

Solvent extraction – principles of ion exchange, paper, thin layer and column Chromatography techniques – Columns, adsorbents, methods, R_f values, McReynold's constants and their uses – HPTLC, HPLC techniques – Adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques: methods, principles and uses.

UNIT IV

Thermo analytical methods:

Principles and applications of Thermogravimetry Analysis (TGA) – Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC). Thermometric titrations.

UNIT V

Electroanalytical techniques and Fluorescence spectroscopy:

Electrochemical sensors, ion sensitive electrodes, glass – membrane electrodes, solid liquid membrane electrodes – ion-selective field effect transistors (ISFETs) – Sensors for the analysis of gases in solution – Amperometric gas sensors – Amperometric titrations: Principles- Apparatus –techniques – applications.

Basic aspects of synchronous fluorescence spectroscopy – Spectral hole burning – flow cytometry – Instrumentation on fluorescence ratio – Fluorimeters (quantization).

References:

1. D.B.Hibbert and J.J. Gooding, Data Analysis for chemistry, Oxford University Press, 2006
2. J.Topping , Errors of Observation and their treatment, Fourth Edn., Chapman Hall, London, 1984
3. R. Stock and C. B. F. Rice, Chromatographic Methods, Chapman and Hall, New York.
4. V.K.Srivastava & K.K. Srivastava, Introduction to Chromatography, S. Chand & Co., New Delhi, 2nd ed,1981.
5. Willard, Merrit, Dean and Settle, Instrumental methods of Analysis CBS Publishers and Distributors, 6th ed., 1986.
6. Skoog, D. A., West, D. M., Holler, F. J., Fundamentals of Analytical Chemistry, 7th edition, Harcourt College Publishers, Singapore. (Pages 523 - 665).
7. A.Sharma, S.G. Schulman, Introduction to Fluoresceence Spectroscopy, Wiley-Interscience. New York,1999
8. C.N.Banwell and E.M.McCash, Fundamentals of Molecular spectroscopy, 4th ed., Tata McGraw-Hill, New Delhi, 1994.
9. Vogel, A. I., Text book of Quantitative Inorganic Analysis, ELBS.
10. Daniel C Harris, Quantitative Chemical Analysis, 4th ed., W. H. Freeman and Company, New York, 1995.
11. S.C.Gupta, Fundamentals of Statistics,6th ed., Himalaya Publ. House, Delhi, 2006.

SEMESTER IV

CORE COURSE XIII - PHYSICAL CHEMISTRY II

UNIT – I

Quantum Chemistry – II & Group Theory

Applications of Wave mechanics, the rigid rotator, harmonic oscillator – Hydrogen atom solution – Shapes and nodal properties of orbitals – Space quantisation – electron spin – Many electron atoms – one electron orbitals – Pauli principle – derminental form of wave function, Helium atom and effective nuclear charge- Approximation methods – Variation methods, application to Hydrogen and Helium atoms– Perturbation method for nondegenerate systems.

Angular momentum in many electron systems – Spin orbit interaction, L-S and j-j coupling schemes.

Atomic Structure Calculation – Self consistent field method for atoms – Hartree and Hartree Fock method for atoms.

Vibrational spectra – symmetry properties of normal molecules – Symmetry co-ordinates – Selection rules for fundamental vibrational transition – IR and Raman activity of fundamentals in CO_2, H_2O, N_2F_2 – The rule of mutual exclusion and fermi resonance.

UNIT - II

Electrochemistry - I

Electrolytic conductance Debye-Huckel-Onsager theory – Debye Falkenhagen and Wien effect. Electrode – electrolyte equilibrium, electrode potential – concentration cells – liquid junction potentials.

Processes at Electrodes- The rate of charge transfer - current density – Butler – Volmer Equation – Tafel equation – Electrical double layer potential – Theory of multiple layers at electrode – electrolyte interfaces – Double layer capacity – Electrokinetic phenomena, Applications: Fuel cells and power storage.

UNIT – III

Electrochemistry - II

Principles and applications of polarography – Instrumentation, Types of cells, advantages of dropping mercury electrode, interpretation of current voltage curves, tests for reversibility, determination of 'n' values (usefulness of Illkovic equation), polarographic maxima, current time curves, Modern developments, Oscillographic polarography, AC polarography – Cyclic Voltammetry, advantages over polarographic techniques – test of reversibility of electron transfer reactions – Chronopotentiometry – apparatus used, advantages over polarography – controlled potential coulometry.

UNIT - IV

Surface Phenomena and Kinetics:

Surface Phenomena: Gibbs adsorption isotherm – solid- liquid interfaces – contact angle and wetting – solid-gas interface – physisorption and chemisorption – Langmuir, BET isotherms – surface area determination. Kinetics of surface reactions involving adsorbed species – Langmuir-Hinshelwood mechanism, Langmuir – Rideal mechanism – Rideal –Eley mechanism. Some interfacial aspects on Micelles, Reverse micelles, Micro emulsions and Membranes.

Chemical Kinetics-II

Application of ARRT to solution kinetics - Effect of solvent and ionic strength, influence of pressure on rates in solution - Enzyme catalysis- Mechanism of single substrate reactions – Michaelis Menton law – Kinetics of processes in micellar and reverse micellar systems.

UNIT – V

Molecular Thermodynamics-II

Third law-thermodynamics-Need for it-Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities at absolute zero – Apparent exceptions to the third law.

Thermodynamics of systems of variable composition – partial molar properties – chemical potential – relationship between partial molar quantities – Gibbs Duhem equation and its applications (the experimental determination of partial molar properties not included).

Thermodynamic properties of real gases – fugacity concept – calculation of fugacity of real gas – Activity and activity coefficient – concept – definition – standard states and experimental determinations of activity and activity coefficient of electrolytes.

References

Text Book

1. F.A. Cotton, Chemical Applications of group Theory, 2nd ed., Wiley Eastern 1971
2. A.K. Chandra, Introductory Quantum Chemistry, 4th ed., Tata McGraw Hill, 1994
3. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1983.
4. J.P. Lowe, Quantum Chemistry, Academic Press, 1978.
5. I.N. Levine, Quantum Chemistry, Allyn and Bacon, 1983.
6. P.W. Atkins, Physical Chemistry, ELBS and Oxford University Press, Oxford, 1983.
7. S.Glasstone, Introduction to Electrochemistry, Affiliated East-West Press, 1968.
8. J.Albery, Electrode Kinetics, Clarendon Press, Oxford Chemical Series, 1979.
9. D.R.Crow, Polarography of Metal Complexes, Academic Press, New York.
10. Daniel C Harris, Quantitative Chemical Analysis, 4th ed., W. H. Freeman and Company, New York, 1995
11. J. Rajaram and J.C.Kuriacose, Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, Shobhan Lal Nagin, New Delhi, 1981.
12. G.W.Castellan, Physical Chemistry, Narosa, New Delhi, 1986.
13. I. M. Klotz and P.M.Rosenberg, Chemical Thermodynamics: Basic Theory and Methods, 3 edn. W.A. Benjamin, New York, 1974.
14. K.J. Laidler, Chemical Kinetics, 2nd ed., Tata McGraw Hill, 1975.
15. A.A. Frost and R.G. Perason, Kinetics and Mechanisms, John Wiley & Sons, New York, 1953.
16. I.Amdur and G.G. Hammes, Chemical Kinetics Principles and Selected Topics, McGraw Hill, New York, 1966.
17. M. Gratzel and K. Kalyanasundaram, Kinetics & Catalysis in Microheterogeneous Systems, Academic Press, New York, 1991.
18. J.I. Steinfeld, J.S.Francisco and W.L. Hase, Chemical Kinetics and Dynamics, 2nd edn, Prentice Hall, New Jersey, 1999.
19. R.K.Dave, Chemical Kinetics, Campus Books, 2000.

CORE COURSE XIV - PHYSICAL CHEMISTRY PRACTICAL-II

Any ten experiments (to be decided by the course teacher) out of the following experiments.

a. Conductometry- Acid- alkali titrations.
b. Cuctometry- Precipitation tritrations.
c. Conductometry- Displacement titrations.
d. Conductometry- Determination of dissociation constant of weak acids.
e. Conductometry- solubility product of sparingly soluble silver salts.
f. Verification of Onsager equation- conductivity method.
g. Determination of degree of hydrolysis and hydrolysis constant of a substance.
h. Potentiometric titrations- Acid alkali titrations.
i. Potentiometric titrations- Precipitation titrations.
j. Potentiometric titrations- Redox titrations.
k. Potentiometry- Determination of dissociation constant of weak acids.
l. Potentiometry- Determination of solubility of silver salts.
m. Potentiometry- Determination of activity and activity coefficient of ions.
n. pH titration of ortho-phosphoric acid.
o. To determine the relative strength of two acids by conductance measurements.
p. To determine the pH of a buffer solution using a quinhydrone electrode.

Reference books (Practical I and II)

1. J.B.Yadav, " Advanced Practical Physical chemistry", 20th edn. GOEL publishing House, Krishna Pakashan Media Ltd., (2001).
2. Findlay's "Practical Physical Chemistry" Revised and edited by B.P. Levitt 9th ed., Longman, London, 1985.
3. J.N. Gurtur and R.Kapoor, "Advanced Experimental chemistry", Vol.I. Chand & Co., Ltd, New Delhi.

ELECTIVE IV : (Green chemistry / Industrial Chemistry)

GREEN CHEMISTRY

UNIT-I

Introduction to green chemistry:

Green chemistry-relevance and goals, Anastas' twelve principles of green chemistry - Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

UNIT-II

Microwave mediated organic synthesis (MAOS):

Microwave activation – advantage of microwave exposure – specific effects of microwave – Neat reactions – solid supports reactions _ Functional group transformations – condensations reactions – oxidations – reductions reactions – multi-component reactions.

UNIT III

Ionic liquids and PTC

Introduction – synthesis of ionic liquids – physical properties – applications in alkylation – hydroformylations – expoxidations – synthesis of ethers – Friedel-craft reactions – Diels-Alder reactions – Knoevengal condensations – Wittig reactions – Phase transfer catalyst - Synthesis – applications.

UNIT IV

Supported catalysts and bio-catalysts for Green chemistry

Introduction – the concept of atom ecomomy – supported metal catalysts – mesoporous silicas – the use of Biocatalysts for green chemistry - modified bio catalysts – fermentations and biotransformations – fine chemicals by microbial fermentations – vitamins and amino acids – Baker's yeast mediated bio-transformations – Bio-catalyst mediated Baeyer-Villiger reactions – Microbial polyester synthesis.

UNIT V

Alternative synthesis, reagents and reaction conditions:

A photochemical alternative to Friedel-crafts reactions - Dimethyl carbonate as a methylating agent – the design and applications of green oxidants – super critical carbon dioxide for synthetic chemistry.

References:

1. Green Chemistry – Environmentally benign reactions – V. K. Ahluwalia. Ane Books India (Publisher). (2006).
2. Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas & Tracy C. Williamson. Second Edition, (1998).
3. Green Chemistry – Frontiers in benign chemical synthesis and processes- edited by Paul T. Anastas & Tracy C. Williamson. Oxford University Press, (1998).
4. Green Chemistry – Environment friendly alternatives- edited by Rashmi Sanghi & M. M. Srivastava, Narora Publishing House, (2003).

OR

INDUSTRIAL CHEMISTRY

UNIT-I

Basic ideas about unit operation – Flow charts – Chemical conversion – Batch versus continuous processing – Chemical process selection – Design – Chemical process control- Chemical process economics – Market evaluation – Plant location – Management for productivity and creativity – Research & Development and its role in chemical industries.

Industrial safety measures – Fire extinguisher, Fire retardant materials – Fire retarding wood – Procedures for handling toxic chemicals

UNIT-II

Fuels.

Fossil fuels- classification and unique features- Coal, Petroleum, natural gas.

Biofuels: Biomass- biodiesel. Nuclear fuels: for various types of nuclear reactors. Hydrogen as fuel in the future, Hydrogen storage materials. Fuel cells – basic principle.

UNIT-III

Oils, fats, waxes and soaps

Introduction-Distinction between oils and fats-properties and its classifications-animal fats and oils-difference between, animal, vegetable and mineral oils-isolation of essential oils and their uses-saponification value-ester value-acid value-iodide value-wijs method – Reichert meissel value-Henher value-elaident test-hydrogenation of oils – Soaps and its manufacture-general consideration in soap making – manufacture of toilet and transparent soaps – oil to be used for soap – cleansing action of soap

Food chemistry: Food processing food preservatives and food additives.

UNIT-IV

Dyes

Introduction-senation of colour- colour and constitution-nomenclature-basic operations in dyeing-classification of dyes according to the mode of application – synthesis, reaction an applications of diphenylmethane dyes-triphenylmethane dyes-phthalein dyes-xanthene dyes-acridine dyes-sulphur dyes-cyanine dyes.

UNIT-V

Polymer Chemistry

Introduction - structure, classification of polymers, polymerisation methods, Importance of polymers, Molecular weight of polymers – Number average and weight average, Determination of molecular weight by osmometry, light scattering, viscosity and sedimentation methods, Kinetics of polymerisation reactions, polycondensation reactions, ionic and free radical polymerisation, copolymersation - coordination polymers, Conducting polymers.

References

1. Chemical Process Industries – Norrish Shreve, R. and Joseph A. Brink Jr. McGraw Hill, Industrial Book Company, London.
2. Production and Properties of Industrial Chemicals – Brain A. C. S. Reinhold – New York.
3. Petroleum Products Hand Book. Guthrie V., McGraw Hill, Tokyo.
4. Industrial Chemistry (Including Chemical Engineering) – B. K. Sharma (10th Edition)
5. Outlines of Chemical Technology – For the 21st Century – M. Gopala Rao & Matshall Sittig (3rd Edition)
6. Source Book on Atomic Energy by S. Glasstone
7. Charles E. Carraher, Polymer chemistry, 6th edn, Marcel Dckker, Brijbasi Art Pvt.Ltd, 2003.
8. F.W.Billmeyer, Jr., A Text Book of Polymer Science, John Wiley and Sons, New York, 1971.
9. V.R.Gowariker, N.V. Viswanathan and Jayadev Sreedhar, Polymer Science, New Age Publishers,New Delhi, 1986.

ELECTIVE V (Chemistry of Nanoscience & Nanotechnology)

Chemistry of Nanoscience and Nanotechnology

UNIT – I

Nanomaterials – An Introduction & Synthetic methods

Definition of nanodimensional materials - Historical milestones - unique properties due to nanosize,Quantum dots, Classification of Nanomaterials .General methods of synthesis of nanomaterials – Hydrothermal synthesis,Solvothermal synthesis,Microwave irradiation, sol – gel and Precipitation technologies, Combustion Flame-Chemical Vapor Condensation Process, gas Phase Condensation Synthesis,Reverse Micelle Synthesis, Polymer – Mediated Synthesis, Protein Microtube – Mediated SynthesisSynthesis of Nanomaterials using microorganisms and other biological agents, Sonochemical Synthesis, Hydrodynamic Cavitation.

Inorganic nanomaterials – Typical examples –nano TiO2 / ZnO/CdO/CdS ,

Organic nanomaterials – examples – Rotaxanes and Catenanes

UNIT – II

Techniques for Characterisation of nanoscale materials: Principles of Atomic force microscopy (AFM)-Transmission electron microscopy (TEM)-Resolution and scanning transition electron microscopy (STEM) Scanning Tunneling Microscopy (STM) Scanning nearfield optical microscopy (SNOM),Scanning ion conductance microscope, scanning thermal microscope, scanning probe microscopes and surface plasmon spectroscopy.

UNIT III

Reactions in Nanospace / Nanoconfinement / Nanocapsules- Cavitands, Cucurbiturils, Zeolites, M.O.Fs, Porous silicon, Nanocatalysis.

UNIT – IV

Carbon Clusters and Nanostructures

Nature of carbon bond – New carbon structures – Carbon clusters: Discovery of C_{60} – Alkali doped C_{60} – Superconductivity in C_{60} – Larger and smaller fullerenes. Carbon nanotubes: Synthesis – Single walled carbon nanotubes – Structure and characterization – Mechanism of formation – Chemically modified carbon nanotubes – Doping – Functionalizing nanotubes –Application of carbon nanotubes. Nanowires – Synthetic strategies – Gas phase and solution phase growth – Growth control – Properties.

UNIT V

Nanotechnology and nanodevices:

DNA as a nanomaterial, DNA – knots and junctions, DNA – nanomechanical device designed by Seeman. Force measurements in simple protein molecules and polymerase – DNA complexes. Molecular recognition and DNA based sensor. Protein nano array, nanopipettes, molecular diodes, self assembled nano transistors, nanoparticle mediated transfection.

References

1. C.N.R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, 2, Wiley – VCH, Weinheim, 2004.
2. C.P. Poole, Jr: F.J. Owens, Introduction to Nanotechnology Wiley Interscience, New Jersey, 2003
3. Kenneth J. Klabunde (Ed), Nanoscale materials in Chemistry, Wiley- Interscience, New York, 2001.
4. T. Pradeep, Nano: The Essentials in understanding nanoscience and nanotechnology, Tata McGraw Hill, New Delhi, 2007.
5. H. Fujita (Ed.), Micromachines as tools in nanotechnology, Springer- Verlag, Berlin, 2003.
6. Bengt Nolting, Methods in modern biophysics, Springer-Verlarg, Berlin, First Indian Reprint, 2004. (Pages 102-146 for Unit II and 147 – 163 for Unit V)
7. H. Gleiter , Nanostructured Materials: Basic Concepts, Microstructure and Properties
8. W. Kain and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John-Wiley R Sons, New York.
9. T. Tang and p. Sheng (Eds), Nano Science and Technology Novel Structures and Phenomena, Taylor & Francis, New York, 2004.
10. A. Nabok, Organic and Inorganic Nanostructures, Artech House, Boston, 2005.
11. Edward A. Rietman, Molecular engineering of Nanosystems, Springer- Verlag, New York, 2001.
12. Home page of Prof. Ned Seeman - http://seemanlab4.chem.nyu.edu/
13. Nano letters - http://pubs.acs.org/journals/nalefd/index.html
    Nanotation - http://www.acsnanotation.org/

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