MANONMANIAM SUNDARANAR UNIVERSITY TIRUNELVELI

PG - COURSES - AFFILIATED COLLEGES

Course Structure for M.Sc. Chemistry

(Choice Based Credit System)
(with effect from the academic year 2017- 2018 onwards)

Sem	Sub.	Subject	Subject Title	Contact	Credits
	No.	Status		Hrs/	
(1)	(2)	(3)	(4)	week	(6)
				(5)	
I	1	Core - 1	Organic Chemistry – I	4	4
	2	Core - 2	Inorganic Chemistry – I	5	4
	3	Core - 3	Physical Chemistry – I	5	4
	4	Elective - 1	Advanced Topics In Chemistry – I	4	4
		Core - 4			
	5	Practical -	Organic Chemistry Practical – I	4	2
		1			
		Core - 5			
	6	Practical -	Inorganic Chemistry Practical – I	4	2
		2			
		Core - 6			
	7	Practical -	Physical Chemistry Practical – I	4	2
		3			
	Subtotal			30	22
II	8	Core - 7	Organic Chemistry – II	5	4
	9	Core - 8	Inorganic Chemistry – II	4	4
	10	Core - 9	Physical Chemistry – II	5	4
	11	Elective - 2	Advanced Topics In Chemistry – II	4	4
		Core - 10			
	12	Practical -	Organic Chemistry Practical – II	4	2
		1			
		Core - 11			
	13	Practical -	Inorganic Chemistry Practical – II	4	2
		2			
		Core - 12			
	14	Practical -	Physical Chemistry Practical – II	4	2
		3			
	Subtotal			30	22

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ORGANIC CHEMISTRY - I

UNIT - I: AROMATICITY AND NOVEL RING SYSTEM

Aromaticity: Benzenoid and non-benzenoid compounds – generations and reactions – sextet theory – MO theory – Huckel's rule – Annulenes and hetero annulenes – Anti and homo aromaticity – Fullerenes.

Novel ring system: Nomenclature of bicyclic and tricyclic systems – structure and synthesis of Adamantane – Congressane – Alternant and non – alternant – Azulene – and sydnones.

UNIT - II: ORGANIC REACTION MECHANISM AND METHODS

Reaction mechanism: Energy diagram of simple Organic reactions – Transition state and intermediate. Kinetic and Thermodynamic requirements of reactions –Baldwin rules for ring closure -Hammond Postulate and microscopic reversibility.

Methods: Kinetic and Thermodynamic control of product formation. Kinetic methods of determination: Rate law – Primary and secondary isotope effect. Non-Kinetic methods of determination: Testing and Trapping of intermediates, Isotopic labeling, Cross–over experiment and stereo chemical evidence.

LFER: Hammett equation – Physical significance of σ and ρ – Applications and Limitations – Taft equation.

UNIT - III: STEREOCHEMISTRY

Concept of chirality: – Enantiotopic, diastereotopic hydrogens and prochiral centres – axial and planar chirality – stereochemistry of compounds containing two dissimilar asymmetric carbons, ansa compounds and para cyclophanes.

R/S notations of Spiranes, allenes and Biphenyl ortho derivatives – E/Z notation of compounds containing one and two double bonds.

Stereospecific and stereoselective synthesis – Methods of Asymmetric synthesis including enzymatic and catalytic process – Cram's rule and Prelog's rule – Cram chelation model and Felkin – Aln model.

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UNIT - IV: REARRANGEMENT REACTIONS

Types of rearrangements: Nucleophilic, electrophilic and Free radical and protrophic reactions.

Mechanism: Nature of migration – migrating aptitude and memory effects, ring enlargement and ring contraction rearrangements.

Reactions: Carbon to carbon migration: Wagner – Meerwein, Pinacol – Pinacolone, Benzil – Benzilic acid, Arndt – Eistert synthesis, Demjanov and dienone-phenol rearrangements.

Carbon to oxygen migration – Baeyer–Villiger, Hydro peroxide and Dakin rearrangements.

Carbon to Nitrogen migration – Lossen, Neber and curtius rearrangements. **Miscellaneous:** Von – Richter rearrangement and Fischer - Indole synthesis.

UNIT - V: REAGENTS IN ORGANIC SYNTHESIS

Gilman's reagent – LDA – DCC – 1,3 – dithane (umpolung synthesis) – Selenium dioxide. Fetizon's reagent – Lemieux – Von Rudloff reagent – Lemieux–Johnson reagent – Woodward and prevost hydroxylation. Merrifield resin – Vaskas catalyst – Wilkinson's catalyst

- 1. P. Sykes, 'A Guide book to mechanism in organic chemistry', Orient Longman, 1989.
- 2. S.M. Mukherji and S.P. singh, 'Reaction mechanism in Organic Chemistry', Macmillan India Ltd, 1978.
- 3. M. Mukerji, S.P. Singh, and R.P. Kapoor, "Organic chemistry", Vol. I and II, Wiley Eastern Ltd., 1985.
- 4. J.March, 'Advanced organic chemistry', Fourth Edition, John Wiley and Sons, Newyork, 2006.
- 5. I.L. Finar, 'Organic Chemistry', Vol I and II, ELBS, fifth Editon, 2001.
- 6. F.A. Carey and R.A Sundberg, 'Advanced Organic Chemistry' (part A and B) plenum publishers, 2000.
- 7. E.S. Gould, 'Mechanism and structure in organic chemistry' Holt, Rinehart and Winston Inc., 1959
- 8. S.H. Pine, 'Organic Chemistry', 5th Edition, Mc Craw Hill International Edition, 1987.
- 9. E.L. Eliel, 'Stereochemistry of Carbon compounds, Mc Craw Hill 1999.
- 10. E.L. Eliel and S.H. Wilen, 'Stereochemistry of organic compounds', John Wiley and sons, Inc., 2003.

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- 11. P.S. Kalsi, 'Stereo chemistry Conformation and mechanism New Age international (p) Ltd., 2000.
- 12. P.Ramesh, 'Basic Principles of organic stereochemistry', Meenu Publications, Madurai, First Edition, 2005.
- 13. D. Nasipuri, 'Stereochemistry of organic compounds Principles and applications', Wiley Eastern Ltd., 1991.
- 14. J.M. Harris and C. Wamser John, 'Fundamentals of organic reaction mechanism Wiley and sons
- 15. F.A Carey, 'Organic Chemistry, Tata Mc Graw Hill, fifth reprint, 2005.
- 16. T.H. Lowry and K.S Richardson,' Mechanism and Theory in Organic Chemistry', Houper and Row Publishers Newyork, 1987
- 17. V.M. Potapov, 'Stereochemistry' Mir Publishers ,1979
- 18. R.O.C.Norman, 'Principles of Organic Synthesis, Chapman Hall, London, 1993.
- 19. Raj K. Bansal, 'Reaction mechanism in Organic chemistry, Tata Mc Graw Hill, Third Editon, 10th reprint, 2005.
- 20. Gurdeep R. Chatwal, 'Reaction mechanism and Reagents in organic chemistry', Himalaya publishing House, Bombay 1992.
- 21. J.N. Gurtu and R. Kapoor, 'Organic Reactions and Reagents', S.Chand and company Pvt. Ltd.,
- 22. Gurdeep Chatwal, 'Organic Chemistry of Natural Products,' Vol.I and II, Himalaya Publishing House, Bombay 1992.
- 23. O.P. Agarwal, 'Chemistry of Natural Products,'Vol I and II, Goel publishing House, Meerut, 1984.
- 24. V.K. Ahluwalia and R.K. Parshar, 'Organic Reaction mechanism,'second Edition , Narosa publishing House,2005.
- 25. H.O. House, 'Modern synthetic Reaction,'Second Edition , W.A. Benjamin, Inc., London, 1972.
- 26. R.K. Mackie, M.M. Smith and R.A. Aitken, 'Guide Book to Organic Synthesis' Second Edition, Longman Seientific and Technical, Singapore, 1990.
- 27. K. Nakanishi, 'Natural Product Chemistry,'Blackie Publications, Vols, I, II, III.
- 28. R.H. Thomson, 'Chemistry of Natural Products Wiley, Newyork, 1996.
- 29. R.T. Morrison and R.N. Boyd, 'Organic Chemistry' sixth Edition, Prentice Hall, 1994.
- 30. Michael B. Smith, 'Organic Synthesis,' Mc Graw Hill international Edition, 1994.
- 31. Bhupinder Mehta, Manju Mehta, Organic Chemistry, PHI Learning, New Delhi, 2011
- 32. Organic chemistry by Clayden, Greeves, Warren & Wothers.
- 33. Organic chemistry by John McMurry.
- 34. Organic chemistry by L.G. Wade. JR.
- 35. Named Organic reactions by Thomas laue & Andreas Plagens.

INORGANIC CHEMISTRY – I

Unit - I: CHEMICAL BONDING

Valence Bond theory: Linear combination of A.O's in hybridization - stereochemistry of the hybrid orbitals - Calculation of s and p characters of equivalence and non-equivalence of hybrid orbitals - **VSEPR theory** - Walsh diagrams - Bent's rule.

M.O. theory – symmetry and overlap in M.O's - σ , π , $\partial \mathbb{D}$ M.O's- phi and mu bonds (Delta and quadrupole bond formation) – M.O. diagrams of hetero nuclear diatomic molecules (CO, NO) and triatomic molecules (BeH₂, CO₂).

Ionic Bond: Lattice energy – Born-Lande equation, Born Haber cycle and numerical problems involving it for the calculation of electron affinity or lattice energy – Kapustinskii equation.

Unit - II: REDOX POTENTIAL AND NON-AQUEOUS SOLVENTS

Redox potential: Applications of redox potential to inorganic reactions - factors affecting redox potential.

Acid-Base - Concept of acids and bases, Hard Soft Acid Base (HSAB) concept, symbiosis in hardening or softening a centre - levelling effect - acid-base strength verses HSAB principle.

Non-aqueous solvents: Classification of protic and aprotic solvents. Self ionization and leveling effect. Reactions in non-aqueous solvents - acid-base reactions, complex formation solvolysis, solvation - reactions in liquid ammonia and liquid SO₂. Use of ionic liquids in synthesis.

Unit - III: SOLID STATE CHEMISTRY

Description of crystal structures: calcite, zinc blende, wurtzite, rutile, fluorite, antifluorite, CsCl, CdI_2 , K_2NiF_4 - spinels and perovskite. Crystal defects in solids - line and plane defects - Point defects - Schottky and Frenkel defects - Non-stoichiometric defects - Colour centres - Solid electrolytes and their applications.

Band theory - optical and electrical properties of semiconductors. Super conductivity - high temperature super conductors, properties and applications - BCS theory - Cooper electrons - Meissener effect and levitation.

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Unit - IV: LANTHANIDES AND ACTINIDES

Correlation of electronic structures, occurrence, extraction from ores and separation methods (Ion exchange and solvent extraction method) and properties of the elements - Chemistry of separation of Pu from U and fission products - Common and uncommon oxidation states - Comparison with transition elements - Lanthanide and actinide contractions - magnetic characteristics of lanthanides and actinides - Similarities between actinides and lanthanides - Use of lanthanide complexes as shift reagents.

UNIT -V: NUCLEAR CHEMISTRY

Atomic nuclei: Nuclear shell structure – nuclear reactions: types, Q-value, threshold energy, cross sections and excitation functions. Direct nuclear reactions – transmutation reactions: stripping and pick-up – high energy reactions: neutron evaporation and spallation – heavy ion reactions – photonuclear reactions. Nuclear fusion and stellar energy – nuclear fission: mass and charge distribution of fission products – fission energy – fission neutrons – theory of nuclear fission – spontaneous fission. Waste disposal and atomic power project in India.

Radio isotopes: Preparation - Analytical applications: radio chromatography, neutron activation analysis, neutron absorptiometry and radiometric titrations.

- 1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic chemistry:* principles Structure and Reactivity, 4th Ed., Harper College Publishers, 1993.
- 2. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Marilo and Manfred Bochman, *Advanced Inorganic Chemistry*, Wiley Interscience Publication, 6th Ed., 1999.
- 3. D.F. Shriver, P.W. Atkins and C.H. Langford, *Inorganic Chemistry*, ELBS, Oxford University Press, 1994.
- 4. N.N. Greenwood and Earnshaw, *Chemistry of the Elements*, Pergamon Press, 2nd Edition, 1997.
- 5. K.F. Purcell and J.C. Kotz, *Advanced Inorganic Chemistry*, Saunders Golden Publishers.
- 6. B.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley and Sons Ltd. 2nd Ed., 1983.
- 7. J.D. Lee, Concise Inorganic Chemistry, ELBS, 2006.
- 8. A. R. West, *Solid State Chemistry and its Application*, John Wiley & Sons, (Asia), 1998.

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- 9. T. Kutty, J. Tareen, *Fundamentals of Crystal Chemistry*, University Press, 1st Ed., 2001.
- 10. L.V. Azaroff, Introduction to Solids, Tata McGraw Hill Publishing Ltd., India, 1989.
- 11. C. Kittel, *Introduction to Solid State Physics*, Wiley Eastern Ltd., 5th Ed., 1993.
- 12. H.V. Keer, *Principles of the Solid State*, Wiley Eastern Ltd., 1993.
- 13. D.K. Chakrabarthy, Solid State Chemistry, New Age International.
- 14. A.F. Wells, *Structural Inorganic Chemistry*, Oxford Science Publication, London, 1979.
- 15. B. Sahoo, N. C. Nayak, A. Samantaray, P.K. Pujapanda, *Inorganic Chemistry*, PHI Learning, New Delhi, 2012.
- 16. Samuel Glasstone, Source Book of Atomic Energy, East West Pvt.Ltd., 1969.
- 17. H.J. Arnikar, *Essentials of Nuclear Chemistry*, Wiley Eastern Ltd., 4th Edition ,2000.
- 18. G. Friedlander, J.W. Kennedy, E.S. Macies and Julian Malcolm, *Nuclear and Radiation Chemistry*, A. Wiley Interscience publication, 1981.

PHYSICAL CHEMISTRY - I

UNIT-I Thermodynamics

Concepts of partial molar properties – partial molar free energy, chemical potential, partial molar volume and its significance. Gibbs-Duhem equation, Gibbs-DuhemMargulus equation. Determination of partial molar volume: Graphical method, intercept method and apparent molar volume method. Concept of fugacity; Determination of fugacity by graphical method and compressibility factor method. Concept of Activity and activity coefficients. Determination of activity and activity coefficients for non-electrolytes.

UNIT-II Phase Rule

Phase rule and Lever rule-Derivation of phase rule from the concept of chemical potential. Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids.

Thermodynamics of irreversible processes

Thermodynamics of irreversible processes with simple examples. Entropy productionrate of entropy production, entropy production in chemical reactions. Onsager reciprocal relations- validity and verification. Thermoelectric phenomena- Electro kinetic and thermo mechanical effects. Application of irreversible thermodynamics to biological and non-linear systems.

UNIT-III 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 – decline of old quantum theory. Schrödinger equation – postulates of quantum mechanics – operator algebra: linear operator, Hermitian operators, eigenfunctions and eigenvalues, angular momentum operator – commutation relations and related theorems – orthogonality and normalization.

UNIT IV Statistical Thermodynamics

Thermodynamic probability – probability theorems – relation between entropy and probability (Boltzmann-Planck equation), ensembles, phase space, Ergodic hypothesis, microstates and macrostates, Maxwell-Boltzmann distribution law – partition functions – translational, rotational, vibrational and electronic partition functions. Relationship between partition functions and thermodynamic properties – calculation of equilibrium constants from partition functions – heat capacities of monatomic crystals – Einstein theory and Debye theory. Quantum statistics – Bose-Einstein (B.E.) and Fermi-Dirac

(F.D.) distribution equations – comparison of B.E. and F.D. statistics with Boltzmann statistics. Concept of negative Kelvin temperature.

UNIT-V MOLECULAR SPECTROSCOPY (Introduction and Rotational Spectroscopy)

Electromagnetic radiation: quantization of energy; rotational, vibrational, and electronic energy levels and transitions in molecules; regions and representation of spectra. Width of spectral lines-collision broadening, Doppler broadening, Heisenberg uncertainty principle. Intensity of spectral lines-selection rules and transition probability, transition moment integral. Diatomic molecules as rigid rotors: rotational energy levels, intensity of spectral lines, selection rules, effect of isotopic substitution. Diatomic molecules as non-rigid rotors: rotational transitions. Rotational spectra of linear and symmetric top polyatomic molecules.

- 1. P. W. Atkins Physical Chemistry, 6th Edtion Oxford, 1998.
- 2. Y. V. C. Rao, An Introduction to Thermodynamics, Wiley Eastern, 1993.
- 3. Physical Chemistry, R.S.Berry, S.A.Rice and J.Ross, Oxford, 2001.
- 4. M. Ladd, Introduction to Physical Chemistry, Cambridge, 1998.
- 5. D. A. McQuarrie and J. D. Simon, Physical Chemistry, A molecular Approach, Viva, 1998.
- 6. F. W. Sears & G. L. Salinger, Thermodynamics, Kinetic Theory & Statistical Thermodynamics, Narosa, 1986.
- 7. D.A. McQurrie and J.D. Simon, Physical Chemistry, A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999.
- 8. S.H. Maron and J.B. Lando, Fundamentals of Physical chemistry, MacMillan Publishers, New York, 1974.
- 9. I. N. Levine: Quantum Chemistry, Prentice Hall India, 1994.
- 10. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, 1998.
- 11. A. K. Chandra, Introductory Quantum Chemistry; 4th Ed., Tata McGraw Hill, Noida, 1994.
- 12. D. A. Mcquarrie, Quantum Chemistry; University Science Books, Sausalito, 2008.
- 13. I. N. Levine, Quantum Chemistry; 5th Ed., Prentice Hall, New Jersey, 2000.

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- 14. R. K. Prasad, Quantum Chemistry; 4th Ed., New Age International Publishers, New Delhi, 2014.
- 15. K. Rajaram and J.C. Kuriacose, Thermodynamics For Students of Chemistry, 2nd Edition, S.L.N. Chand and Co, Jalandhar, 1986.
- 16. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry Classical, Statistical and Irreversible; Pearson Education, New Delhi, 2013.
- 17. I.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, 6th edition, W.A.Benjamin Publishers, California, 1972.
- 18. M.C. Gupta, Statistical Thermodynamics, New Age International, Pvt., Ltd., New Delhi, 1995.
- 19. D.A. McQurrie and J.D. Simon, Physical Chemistry, A Molecular Approach, Viva Books Pvt. Ltd., New Delhi, 1999.
- 20. R.P. Rastogi and R.R. Misra, Classical Thermodynamics, Vikas Publishing, Pvt., Ltd., New Delhi, 1990.
- 21. Horia Metiu, Physical Chemistry, Thermodynamics; Taylor and Francis, Singapore, 2006.
- 22. C. N. Banwell, Fundamentals of Molecular Spectroscopy; 4th Ed., McGraw Hill Education, Noida, 1994.
- 23. G. M. Barrow, Introduction to Molecular Spectroscopy; McGraw Hill, New York, 1964.

ADVANCED TOPICS IN CHEMISTRY – I

(Semester - I)

Unit - I: Green Chemistry

Need of green Chemistry – Anastas twelve principles of green Chemistry – Concept of atom economy – Green Reactions – Microwave assisted reactions – Superiority of microwave exposure over thermal reactions – Functional groups – Transportation – Condensation reactions – Oxidation and reduction reactions.

Unit - I: Nano Chemistry

Definition and terminology of Nano particles and Nano structural materials – Synthesis of Nano particles by Physical approaches (Laser ablation, evaporation and sputtering) and Chemical approaches (reduction of metal ions by Citrate and borohydride, Polyol synthesis) green synthesis – Optical and electronic properties of Nano materials.

Unit - III : Applied Electro Chemistry

Principles of Corrosion – Definition – Cost of Corrosion – Electro chemical principles of Corrosion – Corrosion monitoring methods - Coupan (weight loss) – electrical resistance – gasometric – Potentiodynamic polarisation – impedance – hydrogen permeation – Corrosion inhibition – definition – Classification of inhibitors based on electrode process – mechanism of inhibitor action in acidic medium.

Unit - IV: Analytical Chemistry

Principle and Techniques of GC – MS, HPLC, Cyclic voltammetry, Coulometry and Amprometry.

Theoretical and practical aspects of Colorimetry analysis - Flame emission and Atomic absorption spectroscopy - Advantages of atomic absorption spectrometry over flame photometry.

Unit - V : Industrial Chemistry

Nuclear fuels for various types of Nuclear reactors – Hydrogen as fuel in the future, Hydrogen storage materials – Solar energy – fuel from Sun light – Splitting of water – Hydrogen from Sun light – Hydrogen economy – Fuel cells – batteries – Photovoltaics – Stealing the Sun.

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REFERENCES

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- 2. Green chemistry Designing Chemistry for the environment edited by Paul T. Anastas & Tracy C. Williamson. Second edition. (1998)
- 3. Green chemistry Environment friendly alternatives edited by rashmi sanghi & M.M. Srivastava, Narora Publishing House, (2003)
- 4. Kenneth J. Klabunde, Nanoscale materials in chemistry, John Wiley and sons, Inc. Publication, 2001.
- 5. K.Klabunde and G.Sergeev, Nano chemistry, 2006.
- 6. Guozhong Cao, *Nanostructures and Nanomaterials: Synthesis, Properties and Applications*, Imperial College Press, 2004.
- 7. P.M. Ajayan, L.S. Schadler, P.V. Braun, *Nano composite Science and Technology*, Wiley-VCH, 2003.
- 8. T. Pradeep, *NANO: The Essentials Understanding Nanoscience and Nanotechnology,* Tata McGraw-Hill Publishing Company Limited, New Delhi, 2007.
- 9. C. Brechignac, P. Houdy, M. Lahmani, Nanomaterials and Nano chemistry, Springer 2006.
- 10. An introduction to metallic corrosion and its prevention by Raj Narayanan.
- 11. Vogel's Textbook of Quantitative chemical Analysis by G.H.Jeffery, J. Bassett, J.Mendham, and R.C. Denney, Longman Scientific & Technical, 5th edition, 1989.
- 12. Electro analytical chemistry Basil H. Vassons and Galen W.Ewing, Wiley Interscience publication 1983.
- 13. Chemistry Experiments for instrumental methods Donald T. Sawyer, William R. Heineman, Janice M. Beebe, John Wiley & Sons, 1984.
- 14. D.A. Skoog and D.M.West fundamentals of Analytical Chemistry
- 15. D.A. Skoog Instrumental Methods of Analysis
- 16. Skoog, West, Holler and Crouch Analytical Chemistry An Introduction
- 17. Energy resources and the environment, V.K. Prabhakar, 2001.
- 18. Fundamental Concepts of Applied chemistry, Jayashree Ghosh, S.Chand, 2005

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ORGANIC CHEMISTRY - I

A. Separation of Organic mixture:

- (i) Separation of two component mixture and determination of their physical Constants.
- (ii) Separation and analysis of at least **six** two component mixture. The students are expected to determine the physical constants for both the components as well as their Derivatives.
- (iii) Analysis may be performed in micro (or) macro scale depending upon the Conditions of the laboratory

B. For Class Work Only:

- (1) Separation of Caffeine from Tea / Coffee.
- (2) Separation of green, blue, red inks by TLC method

- 1.F. C. Mann and B. C. Saunders, Practical organic chemistry, Fourth edition, ELBS, 1970.
- 2. A.I. Vogel, A Text book of Practical organic chemistry.
- 3. A.I. Vogel, A Text book of Quantitative Organic Analysis, 1989.
- 4. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Second Edition, Wiley Eastern Ltd., 1990.
- 5. Moore, Dalrympk and Rodig, Experimental methods in organic chemistry, 3rd edition, Saunders College publishing, The Oxford Press, 1982.
- 6. Bassett et.al, A Text Book of Quantitative Inorganic Analysis, ELBS, 1986
- 7. Roberts, Gilbert, Reidwald-Wingrove. An Introduction to Experimental Organic Chemistry, 1969.

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1. Qualitative analysis of inorganic mixture containing two familiar and two less familiar cations Pb, Cu, Bi, Cd, Sb, Zn, Co, Ni, Mn, Ca, Ba, Sr, W, Tl, Te, Se, Mo, Ce, Th, Zr, V, U, Ti and Li.

- 1. G. Svehla, *Vogel's qualitative inorganic analysis*, 7th Edition, Pearson Education India, 2008.
- 2. V. Ramanujan, *Inorganic Semi-micro Qualitative Analysis*, 3rd Edition., National Publishing Company, Chennai, 1990.

PHYSICAL CHEMISTRY -I

I. Conductometry

Conductometric Titrations

- a. Estimation of HCl and AcOH in a mixture
- b. Estimation of NH₄Cl and HCl in a mixture
- c. Conductometry- solubility product of sparingly soluble silver salts.

II. Thermometry

- a. Determination of Solution enthalpy of
 - i. oxalic acid-water
 - ii. ammonium oxalate-water
 - iii. Potassium dichromate-water

III. Kinetics - Acid hydrolysis of ester - comparison of strength of acids.

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ORGANIC CHEMISTRY – II

Unit - I: ULTRAVIOLET, INFRA - RED SPECTROSCOPY, ORD AND CD

UV: The absorption laws – Types of electronic transitions – effect of solvents and Hydrogen bonding on λ_{max} values. – Woodward – Fieser rules to calculate λ_{max} values of conjugated dienes and α,β - unsaturated ketones.

IR: Characteristic IR absorptions of different functional groups – factors influencing absorption of carbonyl and hydroxyl groups – electronic effect and effect of hydrogen bonding, Fermi resonance and Finger print region.

ORD and CD: Optical rotatory dispersion (ORD): Octant rule – alpha - halo ketone rule and their Applications-Circular Dichroism.

Unit-II: Aromatic nucleophilic substitution Reaction and Addition to carbon-carbon multiple bonds and carbon - oxygen double bond.

Aromatic nucleophilic substitution reaction : Unimolecular, Bimolecular and Benzyne mechanisms - Reactivity, effect of substrate, leaving group and attacking nucleophile-typical reaction as oxygen and sulphur as nucleophile - Bucherer and Rosenmund reaction- Smiles rearrangement.

Catalytic hydrogenation - Birch reduction - Dieckmann condensation - Mannich reaction - Wittig reaction - Sharpless asymmetric epoxidation - addition of hydrogen halides to carbon - carbon double bond - addition of boranes, Michael addition (1,2 and 1,4)

Addition of dialkyl groups to triple bonds. Addition of hydrides – LiAlH₄ and NaBH₄.

Unit-III: Reactive intermediates and rearrangements

Carbenes: Generation, stability, structure, and reactivity of carbenes-Wolff rearrangement of acyl carbenes and its synthetic applications.

Nitrenes: Generation, stability, reaction of nitrenes- Mechanism of rearrangements through Nitrene intermediate: Schmidt, Hoffmann, Beckmann rearrangements.

Carbanion: Generation, Structure, Stability and reaction of carbanion-Mechanism of rearrangements involving carbanion as intermediate: Steven, Sommelet-Hauser and Favorski rearrangements.

Aryne: Generation, Structure, Stability, reactions and trapping of aryne- cine substitution.

Unit - IV: ALKALOIDS AND ANTIBIOTICS

Alkaloids: Degradation studies – HEM, Emde and Von – Braun – Structural elucidation and synthesis of Quinine, Morphine, Cocaine, Lysergic acid and Atropine. Synthesis of Reserpine and PaPaverine – Biosynthesis of tyrosine, tryptophan.

Antibioties: Structure and synthesis of penicillin, cephalosporin – C, chloramphenicol and Streptomycin.

Unit - V: VITAMINS AND TERPENOIDS

Vitamins: Structural elucidation, synthesis of vitamins – A_1 , B_1 and C - synthesis of vitamins B_2 , B_6 , D and E.

Terpenoids: Structural elucidation, synthesis of α -Pinene, Camphor, α -Cadinene, Zingiberene and squalene - synthesis of α -Santonin and Gibberelic acid. Bio synthesis of mono and di terpenoids.

- 1. J. March, 'Advanced organic chemistry,' Fourth Edition, John Wiley and sons, New York, 2006.
- 2. R.T. Morrison and R.N. Boyd, 'Organic Chemistry', sixth Edition, Prentice Hall, 1994
- 3. I.L. Finar, 'Organic Chemistry', volume 2, sixth Edition, Pearson Education Inc., Singapore, 2006.
- 4. Y.R. Sharma, 'Fundamentals of Organic spectroscopy'.
- 5. P.S. Kalsi, 'Spectroscopy of organic spectroscopy', second Edition, New Age International Publishers Limited, 1995.
- 6. Jag Mohan, 'Organic Analytical Chemistry Theory and Practice, 'Narosa Publishing House, 2003.
- 7. W.Kemp, 'Organic spectroscopy', Third Edition, Macmillan, 1994.
- 8. S.M. Silverstein, G.V.Bassler and T.C. Morril, 'Spectrometric Identification of organic compounds, sixth Edition, Wiley 2004.

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- 11. V.R. Dani, 'Organic spectroscopy', Tata Mc Graw Hill, 1995.
- 12. J.R. Dyer, 'Application of Absorption spectroscopy, prentice Hall, 1987.
- 13. Pavia, Lampmann, Kriz and Vyuyan, spectroscopy, cengage learning India Private Ltd., First Indian Reprint, 2008.
- 14. D.H. William and R.D. Bower, 'Mass spectrometry principles and Applications,' I. Howe, Mc Graw Hill.
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INORGANIC CHEMISTRY - II

Unit - I: BONDING IN COORDINATION COMPOUNDS

CFT and LFT: Basic features of CFT and LFT. Splitting of the metal d - orbitals in T_d , O_h and square planar symmetries - Jahn-Teller distortion in O_h and T_d complexes - Static and dynamic J.T distortions. Application of CFT: Magnetic Properties - Spectral properties - Spectrochemical series - Kinetic properties. **CFSE**: Calculation of CFSE in O_h and T_d complexes - Contribution of CFSC to M-L bond energy, M-L step-wise stability constants, Hydration energies of M^{n+} - Lattice energy - Preferred stereochemistry - Site selection of the cations in spinel and inverse spinel and OSSE.

MOT: \square -bonding and \square -bonding in O_h complexes - Effect of \square -bonding on the value of Δ (10 Dq). MOT for square planar (16 e⁻) and T_d (18 e⁻) complexes. Application of MOT to explain spectrochemical series.

Unit - II: STABILITY AND REACTIONS OF COORDINATION COMPOUNDS

Stability of complexes - Thermodynamic and kinetic stabilities - stepwise and overall stability constants of the metal complexes - factors affecting stability - chelate and template effects - Determination of stability constants and composition of the complexes: Bjerrum's method, potentiometric determination, spectrophotometric method, ion-exchange method, polarographic method, continuous variation (Job's) method.

Reactions of complexes: Lability – inertness - Ligand substitution reactions of square planar complexes - Trans effect and trans influence - Theories of trans effect - use of trans effect in synthesis of complexes - Substitution reactions in octahedral complexes - acid hydrolysis, base hydrolysis and anation reactions - Electron transfer reactions - Inner sphere and outer sphere processes - complementary and non-complementary reactions.

Unit - III: ELECTRONIC AND INFRARED SPECTROSCOPY

Electronic spectroscopy: Selection rules for electronic transitions - Line width and shape - Hole formalism - LS Coupling and jj coupling schemes and determination of term symbols – Splitting of terms – Orgel and Tanabe Sugano diagrams – Electronic spectra of Ist row transition metal complexes - Evaluation of 10 Dq, β and B' for octahedral d² and d8 systems. Charge transfer spectra - types - Effect of tetragonal distortion and spin - orbit coupling on spectra. Electronic spectra of lanthanide and actinide complexes.

Infrared spectroscopy: Selection rules - calculation of force constants of IR vibrations. Changes in the IR spectra accompanying changes in symmetry upon coordination,

differentiation of coordinated water and lattice water. Application in the study of isomerism - linkage and geometrical isomerism.

Unit - IV: MAGNETIC PROPERTIES OF METAL COMPLEXES

Magnetic properties: Types of magnetism – magnetically diluted and concentrated substances - temperature dependence of magnetic susceptibility of different types of magnetic materials. Paramagnetism and thermal energy – quenching of orbital contribution to magnetic moment by CF – orbital contribution from the excited state through spin – orbit coupling. Mixing of the excited terms with the ground state term through second order Zeeman effect. Magnetic properties of Ist row Transition Metal complexes: comparison of the magnetic properties of O_h, T_d and square planar Fe(II), Co(II), Ni(II) and Cu(II) complexes. Magnetic properties of complexes with A, E and T ground states – magnetic properties of II and III Transition Metal complexes. Application of magnetic moment – oxidation state, structure determination.

Unit V: INORGANIC POLYMERS AND METAL CLUSTERS

Inorganic polymers: General characteristics, degree of polymerization, catenation and heterocatenation - silicates - classification and structure - property correlation - Polyacids - structures of isopoly and heteropoly anions - Polymeric sulphur nitride - Borazines - Phosphazenes - Phosphazene polymers - Boranes and carboranes - Structure and bonding in boranes - Molecular frame work of hydrides of boron skeletal electron pair counting and Wade's rule.

Structure and Bonding of Metal clusters: Dinuclear Clusters: Cu(II) carboxylate, Chromium(II) acetate, and $[M_2Cl_8]^{4-}$ (M = Mo and Re) - Trinuclear Clusters: $[M_3(CO)_{12}]$ (M = Fe, Ru, Os) - Teteranuclear Clusters: $[M_4(CO)_{12}]$ (M = Co, Rh, Ir) - Hexanuclear Clusters: $[Nb_6Cl_{12}]^{2+}$, $[Os_6 (CO)_{18}]^{2-}$ and $[Mo_6Cl_8]Cl_4$ - Capping rule - poly atomic Zintl ions.

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- 16. C.N.R.Rao, Chemical Applications of Infrared Spectroscopy, Academic Press, New york, 1963.
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- 21. T. Pradeep, *NANO: The Essentials Understanding Nanoscience and Nanotechnology*, Tata McGraw-Hill Publishing Company Limited, New Delhi, 2007.
- 22. C. Brechignac, P. Houdy, M. Lahmani, *Nanomaterials and Nano chemistry*, Springer 2006.

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PHYSICAL CHEMISTRY-II

UNIT-I Quantum Mechanics I

Setting up and solving Schrodinger wave equation and arriving solution for Particle in 1D box, Particle in a ring, 3D Rectangular box, 3D cubical box, the harmonic oscillator, the rigid rotator, and the hydrogen atom. Degeneracy and degenerate wave functions, Quantum mechanical tunnelling. Shapes and nodal properties of orbitals – Space quantisation.

UNIT-II Quantum Mechanics II

Electron spin, Anti symmetry and Pauli's exclusion principle – Slater determinantal wave functions. Approximation methods-The Variation theorem; Linear Variation Principle, Perturbation theory. Applications of Variation Method and Perturbation Theory to the Helium atom. Born-Oppenheimer approximation, VB and MO theory, for H₂+ molecular ion and H₂ molecule problems, Hartree Fock Self consistent field method for Helium atom. Hückel Molecular Orbital Theory and its application to ethylene, butadiene and benzene.

UNIT - III Electrochemistry - I

Arrhenius theory, Derivation and Validity of Debye-Huckel Theory, Debye-Huckel-Onsager conductance equation, Deviations from Onsager equation. Debye-Falkenhagen effect and Wien effect. Activity of electrolytes, Determination of activity and activity coefficient using Debye-Huckel theory. Debye-Huckel Limiting law, Debye-Huckel-Bronsted equation. Definition and Determination of Transference number. Abnormal transference number. Electrified interfaces-Lipmann equation derivation. Electrical Double Layer, Structure of electrical double layer Helmholtz-Perrin, Guoy-Chapmann and Stern models of electrical double layer- Applications and limitations. Kinetics of electrode reaction-Butler-Volmer equation, Tafel equation.

UNIT - IV Electrochemistry - II

The Poisson-Boltzmann equation and its solutions. Electrocapillary phenomena-Zeta potential and its applications. Electrophoresis and related phenomena- The electro viscous effect, sedimentation Potential, Electrophoresis. Effect of electrical double layer-Electrocapillarity, Double layer capactance Corrosion and passivation of metals – Pourbaix diagram – Evans diagram – fuel cells – primary and secondary fuel cells – electrodeposition – principle and applications.

Principles and applications of Polarography–Instrumentation, 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

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polarographic techniques – Test of reversibility of electron transfer reactions – Chronopotentiometry – apparatus used, advantages over polarography – controlled potential coulometry.

UNIT-V Photochemistry and Radiation Chemistry:

Photochemistry: Introduction. Laws of photochemistry, Quantum yield and its determination. Physical properties of electronically excited molecules: excited state dipole moment, acidity constant and redox Potentials. Photophysical processes in electronically excited molecules: Jablonski diagram – Intersystem system crossing internal conversion, fluorescence, phosphorescence and other deactivation processes. Photosensitisation chemiluminescence and bioluminescence - Stern-Volmer equation and its applications – mechanisms of quenching – electron transfer – energy transferexperimental techniques in photochemistry –chemical actinometers.

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- Dosimetry and dosimeters in radiation chemistry- application of radiation chemistry.

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- 2. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, 1998.
- 3. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford,1982.
- 4. P. W Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
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- 6. Murrel, Kettle and Tedder: Valency Theory, ELBS, London, 1966.
- 7. R. McWeeney: Coulson's valence, Oxford-ELBS(3rd ed.) 1976.
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- 10. A. K Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill, 1988.
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- 18. Fundamentals of Photochemistry, K.K. Rohatgi Mukhergee, Wiley Eastern Limited, 1986.
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- 20. Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall, India, New Delhi, 1st Edition, 1972.
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- 22. G.Hughes, Radiation Chemistry, Oxford University Press, 1973.
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ADVANCED TOPICS IN CHEMISTRY - II

UNIT I: Forensic and computer applications in Chemistry

Forensic science: Finger printing, forensic serology, hair and fiber analysis, explosive residue, glass comparisons, drug analysis, bullet and cartridge analysis.

Introduction of computer: molecular modelling simulation and animation. World Wide Web and Chemical Databases on internet, Techniques of information search, Chemsketch and Chemdraw.

UNIT -II: Applications of nanomaterials

Applications of nanomaterials: Applications in catalysis - Organic transformations and fuel cells - Environmental application - Water purification, air purification - Nano particles as sensors - **Nanocomposites** - Polymer-based Nanocomposites - Polyamide/clay Nano composites - Synthesis, characterization and properties of Nylon 6 - clay hybrid - Polystyrene/clay Nanocomposites - syndiotactic polystyrene/clay Nano composites, properties. Poly(butylenes terephthalate) (PBT) based nano composites. Bio-Nanocomposites- properties and applications.

UNIT III: Industrial polymer

Important industrial polymers – synthesis and applications of poly tetra flouro ethylene (TEFLON), ion exchange resins. Synthetic route, structure and applications of engineering plastics - Acrylonitrile butadiene styrene (ABS), Poly amides (PA), Poly ethylene terephthalate (PET), Polyphenylene Oxide (PPO), Poly sulphone (PSU), Poly ether ether ketone (PEEK), Poly amides, Poly phenylene sulphide (PPS).

UNIT IV: Medicinal chemistry

Drug Discovery, Design and development: Identification of diseases and corresponding targets, Bio assays and leads. Streochemistry and solubility issues in drug design.

Structure Activity Relationship (SARS): Changing size and shape- introduction of new substituents. Quantitative structure activity relationships (QSARS), Lipophilicity – electronic and steric effects- Hansch Analysis – Top liss 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 V: Bio-organic chemistry:

Characteristics of enzymes- mechanism of enzyme action- chymotrypsin- antibodies of enzymes- biological energy- ATP, NADH, NADPH, FADH₂ as electron carriers- Co – enzyme A as universal carriers of acyl groups- glycolysis- citric acid cycle- urea cycle – Link between glycolysis and citric acid cycle- lipid metabolism- biological oxidation- bio metic chemistry cyclodextrins- Calixarenes as enzyme model.

- 1. Bell, Suzanne, Forensic Chemistry, 1st Edition, 2006, Prentice Hall.
- 2. Jackson, Andrew R.W and Julie M.Jackson, Forensic Science, 2004, 1st Edition Prentice Hall.
- 3. Khan, Javed, Kennedy, Thomas J., Christian, Jr. Donnell, Basic Principles of Forensic Chemistry 2009, Human Press.
- 4. W.G.Eckert, Introduction to Forensic Sciences, Second Edition, Elsevier, New York, 1992.
- 5. N.E.Genge, The Science of Crime Science Investigation: The forensic Casebook, Ballentine Books, New York 2002.
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- 9. ChemSketch 5.0 User's Guide, Advanced Chemistry Development, (2001).
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- 12. T.Pradeep, Nano: The Essentials in understanding nanoscience and nanotechnology, Tata Mcgraw Hill, New Delhi, 2007.
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- 14. Nano letters http://pubs.acs.org/journals/nalefd/index.html, Nanotation http://www.acsnanotation.org/, Home page of Prof.Ned Seeman-http://seemanlab4.chem.nyu.edu,
- 15. F.W.Bill Meyer, Text book of polymer science, III Edition, John Willey and sons, New York.
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- 21. Progress in preparation, processing and applications of polyaniline. Progress in polymer Science (2009) 783 810.
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- 23. Fundamentals of medicinal chemistry by Gareth Thomas, John Wiley & sons: chichester, 2003.
- 24. Medicinal chemistry: An introduction Gareth Thomson, Wiley- Interscience, 2nd edition, 2008.
- 25. An introduction to Medicinal chemistry by graham L.Patric, Oxford university press, USA, 3rd edition, 2005.
- 26. The Organic chemistry of Drug Design and Drug Action by Richard B. Silverman, Academic press, 2nd edition, 2004.
- 27. Designing organic synthesis: The Disconnection Approach by Stuart Warren, Wiley, 2nd edition, 1984.
- 28. Asymmetric Synthesis by H.B.Kagan, Thieme Medical Publishers, 2003.
- 29. Advanced Organic Chemistry: Part-A and Part-B, Francis A.Carey and Richard B.Sundberg, Springer, 5th Edition, 2007.
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- 31. F.S. Gould, Mchanism and structure in organic chemistry, Holt, New York, 1959.
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ORGANIC CHEMISTRY PRACTICAL - II

A.Estimation

- (i) Estimation of phenol
- (ii) Estimation of aniline
- (iii) Estimation of ascorbic acid

B.List of single stage preparations:

- (i) Preparation of 1,2,3,4 –Tetrahydro carbazole from cyclohexanone.
- (ii) Preparation of Resacetophenone from Resorcinol.
- (iii) Preparation of p-benzoquinone from hydroquinone.
- (iv) Preparation of Bis-2-Naphthol.
- (v) Preparation of Di Benzylidene acetone.
- (vi) Preparation of anthraquinone from anthracene
- (vii) Preparation of benzophenone oxime from benzophenone
- (viii) Preparation of Nerolin from β-Naphthol
- (ix) Preparation of anthranilic acid from Phthalimide
- (x) Preparation of Benzilic acid from Benzil

Note: Each student is expected to submit both Crude and recrystallized samples of the preparation during their regular practical for evaluation at the time of practical examinations.

C. For Class Work Only:

- 1. Download the following spectra from **internet** and give interpretation.
- I. Differentiate the following pair by UV- spectra
 - (a) Trans stilbene and its cis isomer.
 - (b) Vinyl methyl ketone and acetone.
 - (c) Vinyl methyl ketone in two solvents such as n-Hexane and alcohol.
- II. Differentiate the following pair by IR spectra
 - (a)para and ortho hydroxy benzoic acid.
 - (b) p-nitro and p-amino acetophenone.
 - (c) Maleic acid and fumaric acid.
- (2) Separation of Caffeine from Tea / Coffee.

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- 3. A.I. Vogel, A Text book of Quantitative Organic Analysis, 1989.
- 4. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Second Edition, Wiley Eastern Ltd., 1990
- 5. Moore, Dalrympk and Rodig, Experimental methods in organic chemistry, 3rd edition, Saunders College publishing, The Oxford Press, 1982.
- 6. Bassett et.al., A Text Book of Quantitative Inorganic Analysis, ELBS, 1986.
- 7. Roberts, Gilbert, Reidwald-Wingrove An Introduction to Experimental Organic Chemistry, 1969.

MSU / 2017-18 / PG-Colleges / M.Sc. (Chemistry) / Semester-II / Ppr. No.12 / Practical 5 INORGANIC CHEMISTRY PRACTICAL - II

A. Analysis of Mixture of Cations by Complexometric titrations

- 1. Estimation of Cu(II) by EDTA titration in the presence of either Pb(II) or Ba(II) (Sepearation of Pb(II) or Ba(II) by precipitation).
- 2. Estimation of Zn(II) by EDTA titration in the presence of either Pb(II) or Ba(II) (Sepearation of Pb(II) or Ba(II) by precipitation).
- 3. Estimation of Ca(II) and Pb(II) in a mixture by EDTA titration (Selective titration by control of pH).
- 4. Estimation of Cr(III) and Fe(III) in a mixture by EDTA titration (Kinetic masking).
- 5. Estimation of Mg(II) and Mn(II) in a mixture by EDTA titration (Demasking by F^-)
- 6. Estimation of Pb and Sn in Solder alloy by EDTA titration (Demasking by F-).
- 7. Estimation of Ca(II) ion in an antacid or diet supplement pill by EDTA titration (Substitution titration).

B. Photocolorimetric Analysis of Cations (Course work only)

Estimation of Fe, Ni, Cr, Mn, Cu and NH₄⁺. (Any four experiments)

- 1. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, *Vogel's Textbook of quantitative chemical analysis*, Longman Scientific and Technical, 5th Ed., England, 1989.
- 2. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, *Fundamentals of Analytical Chemistry*, 8th Ed., Brooks/Cole-Thomson Learning, USA, 2004.
- 3. I.M. Kolthoff, V.A. Stenger, *Volumetric Analysis*, 2nd Ed., Interscience Publishers, New York, 1947.

PHYSICAL CHEMISTRY PRACTICAL-II

I Conductometric experiments

- (i) Estimation of K₂SO₄ using BaCl₂
- (ii) Estimation of CH₃COOH and CH₃COOONa in a Buffer solution.
- (iii) Determination of Dissociation constant of a weak acid

II Distribution law

- (i) Distribution of Iodine between two immiscible solvents & Study of the equilibrium constant of the reaction $KI + I_2 \rightarrow KI_3$
- (ii) Distribution of benzoic acid between two immiscible solvents

III Thermometry

Determination of Solution enthalpy of

- (i) Benzoic acid-water
- (ii) Napthalene-Tolune
- **IV Kinetics** Study of Kinetics of KI K₂S₂O₈ system.
