List of New Course(s) Introduced

Department : *Chemistry*

Programme Name : *B.Sc.*

Academic Year : 2020-21

List of New Course(s) Introduced

Sr. No.	Course Code	Name of the Course
01.	CBT-11	Organic Chemistry IV
02.	CBL-11	Organic Chemistry IV Practical
03.	CBT-12	Physical Chemistry V
04.	CBL-12	Physical Chemistry V Practical
05.	DSE-1 THEORY	Discipline Specific Elective Theory-1
06.	DSE-1 PRACTICAL	Discipline Specific Elective Practical-1
07.	DSE-2 THEORY	Discipline Specific Elective Theory-2
08.	DSE-2 PRACTICAL	Discipline Specific Elective Practical-2
09.	CBT-13	Inorganic Chemistry IV
10.	CBL-13	Inorganic Chemistry IV Practical
11.	CBT-14	Organic Chemistry V
12.	CBL-14	Organic Chemistry V Practical
13.	DSE-3 THEORY	Discipline Specific Elective Theory-3
14.	DSE-3 PRACTICAL	Discipline Specific Elective Practical-3
15.	DSE-4 PROJECT	Dissertation/ Project work followed by seminar

Minutes of Meetings (MoM) of Board of Studies (BoS)

Academic Year : 2020-21

School : *School of Studies of Physical Science*

Department : *Chemistry*

Date and Time : *Nov. 03, 2017 – 11:30 AM*

Venue : *Meeting room*

The scheduled meeting of member of Board of Studies (BoS) of Department of Chemistry, School of Studies of Physical Science, Guru Ghasidas Vishwavidyalaya, Bilaspur was held to design and discuss the structure and scheme of examination of Integrated UG/PG, M. Sc. Chemistry syllabi.

The following members were present in the meeting:

1. Prof. Bali Ram (External Expert Member BoS, Dept. of Chemistry, BHU, Varanasi)
2. Prof. G. K. Patra (Member BoS, Dept. of Chemistry)
3. Dr. Charu Arora (HOD, Associate Prof., Dept. of Chemistry-cum Chairman, BOS)
4. Dr. Arti Srivastava (Member BoS, Assistant Professor, Dept. of Chemistry)

Following points were discussed during the meeting

1. Draft prepared to revise course structure and scheme of examination in the light of UGC directives (as per CBCS Scheme) to be implemented from 2018-19.
2. Elective paper Advanced Quantum and Computational Chemistry (CMT-405) has been incorporated in M.Sc. IV sem.
3. The core paper Organic Chemistry-IV (CBT-503) of B.Sc.-Vth sem has been interchanged with core paper Physical Chemistry-IV (CBT-601) to justify semester wise teaching load.

The following new courses were introduced in the B. Sc. and M. Sc.:

- B. Sc. CBCS scheme

CBT-11	Organic Chemistry IV
CBL-11	Organic Chemistry IV Practical
CBT-12	Physical Chemistry V
CBL-12	Physical Chemistry V Practical
DSE-1 THEORY	Discipline Specific Elective Theory-1
DSE-1 PRACTICAL	Discipline Specific Elective Practical-1
DSE-2 THEORY	Discipline Specific Elective Theory-2
DSE-2 PRACTICAL	Discipline Specific Elective Practical-2
CBT-13	Inorganic Chemistry IV
CBL-13	Inorganic Chemistry IV Practical
CBT-14	Organic Chemistry V
CBL-14	Organic Chemistry V Practical
DSE-3 THEORY	Discipline Specific Elective Theory-3
DSE-3 PRACTICAL	Discipline Specific Elective Practical-3

DSE-4 PROJECT Dissertation/ Project work followed by seminar

- Advanced Quantum and Computational Chemistry (CMT-405)

Signature of HOD

अध्यक्ष/Head
रसायन शास्त्र विभाग
Deptt. of Chemistry
गुरु घासीदास विश्वविद्यालय,
Guru Ghasidas Vishwavidyalaya,
बिलासपुर 495009 (छ.ग.)
Bilaspur 495009 (C.G.)

Scheme and Syllabus

SUMMER Internship: 15 days			**Swayam Swachhta / NSS / Industrial/ others**	**2**	**100**
V	Core-11	CBT-11	Organic Chemistry IV	4	4
	Core -11 Practical	CBL-11	Organic Chemistry IV: Practical	2	4
	Core -12	CBT-12	Physical Chemistry-V	4	4
	Core -12 Practical	CBL-12	Physical Chemistry-V: Practical	2	4
	Discipline Specific Elective (DSE-1)	DSE-1-THEORY	DSE-I : Theory	4	4
	DSE-1 - Practical	DSE-1-LAB	DSE-I: Practical	2	4
	Discipline Specific Elective (DSE-2)	DSE-2-THEORY	DSE-II : Theory	4	4
	DSE-2 - Practical	DSE-2-LAB	DSE-II: Practical	2	4
			TOTAL	24	32
VI	Core-13	CBT-13	Inorganic Chemistry IV	4	4
	Core -13 Practical	CBL-13	Inorganic Chemistry IV: Practical	2	4
	Core -14	CBT-14	Organic Chemistry V	4	4
	Core -14 Practical	CBL-14	Organic Chemistry V: Practical	2	4
	Discipline Specific Elective (DSE-3)	DSE-3-THEORY	DSE-III : Theory	4	4
	DSE-3 - Practical	DSE-3-LAB	DSE-III: Practical	2	4
	Discipline Specific Elective (DSE-4) + DSE-4 – Practical **Or** Dissertation/ Project work followed by seminar	DSE-4-Project	Dissertation/ Project work followed by seminar	4+2=6 **Or** 5+1=6	8
			TOTAL	24	32
			TOTAL CREDITS	**152 + 4 (SI)**	

As per UGC CBCS guidelines, University / departments have liberty to offer GE and SEC courses offered by one department to students of other departments. The No. of GE course is four. One GE course is compulsory in first 4 semesters each.
Minimum One Skill Enhancement course shall be proposed by each department. (4 credits) [4 L or 2L + 2P or 1L + 3P or 3L + 1T] 1P = 2 hours

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Semester V

CHEMISTRY-C XI: ORGANIC CHEMISTRY-IV (CBT-11)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Methods of Determining Reaction Mechanism: Mechanism of bonds breaking and formation. Inter and intra-molecular migration of groups, crossover experiments, exchange with solvents, importance reactive intermediates. Isotopic substitution in a molecule: primary and secondary kinetic isotope effects - their importance in mechanistic studies.

Chemistry of reaction intermediates: Preparation, reactions and stability of carbenes, nitrenes and arynes.

Molecular Rearrangements: Favourskii rearrangement, Demzov rearrangement. Beckmann, Hofmann, Lossen, Curtius and Wolff rearrangements, Baeyer-Villiger oxidation.

Reagents and reactions in Organic Synthesis: Reducing agents: lithium aluminium hydride, sodium borohydride, Birch reduction. Oxidizing agents: Osmium tetraoxide, Woodward & Prevorst oxidation and m-Chloroperbenzoic acid. Hydroboration,

Ultra-Violet Spectroscopy: Electromagnetic radiation, UV Spectroscopy – Electronic transitions, auxochromes, chromophores, bathochromic and hypsochromic shift, Wood words-Fieser rule for calculating λ_{max} for conjugated dienes and α,β-unsaturated aldehydes and ketones. Interpretation of UV spectra.

Infrared Spectroscopy: Vibration modes and bond stretching. Absorption of common functional groups, Factors affecting vibrational frequency, effects of Hydrogen bonding. Fingerprint region and interpretation of IR spectra.

Books Recommended

1. *"Organic Chemistry"*, I. L. Finar, [Vol. I, 6th Edition (1973), Reprinted in 1980 & Vol. II, 5th Edition (1975), Reprinted in1996], ELBS and Longman Ltd., New Delhi.
2. *"A Guide Book to Mechanism in Organic Chemistry"*, P. Sykes, 6th Edition (1997), Orient Longman Ltd., New Delhi.
3. *"Organic Chemistry"*, R. T. Morrison and R. N. Boyd, 6th Edition (1992), Prentice-Hall of India (P) Ltd., New Delhi.
4. *"Organic Chemistry"*, S. M. Mukherji , S. P. Singh, and R. P. Kapoor, 1st Edition (1985), 5th Reprint (1999), New Age International (P) Ltd.Publishers, New Delhi.
5. "*Organic Chemistry*", J. Clayden, N. Greeves, S. Warren, and E. Wothers, Oxford Univ. Press, Oxford (2001).
6. "*Organic Chemistry*", G. Solomon, Willey Inida, Paper Back, 9th Edition.
7. "*Modern Organic Chemistry*", M. K. Jain and S. C. Sharma, Vishal Publishing CO. Jalandhar, India, 4th Edition (2012).

CHEMISTRY PRACTICAL-C XI ORGANIC CHEMISTRY IV LAB (CBL-11)

60 Lectures

1. Functional group test for nitro, amine and amide groups.
2. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols , carbonyl compounds and esters)

Reference Books:

1. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry 5th Ed., Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
4. Ahluwalia, V.K. &Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

CHEMISTRY-C XII: PHYSICAL CHEMISTRY-V (CBT-12)

(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

Quantum Chemistry

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution

functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.

Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH_2, H_2O) molecules. Qualitative MO theory and its application to AH_2 type molecules.

Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.

Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence.

Reference Books:

- Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
- Chandra, A. K. Introductory Quantum Chemistry Tata McGraw-Hill (2001).
- House, J. E. Fundamentals of Quantum Chemistry 2nd Ed. Elsevier: USA (2004).
- Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005).
- Kakkar, R. Atomic & Molecular Spectroscopy, Cambridge University Press (2015).

CHEMISTRY PRACTICAL-C XII PHYSICAL CHEMISTRY V LAB (CBL-12)

60 Lectures

UV/Visible spectroscopy

I. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
III. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

Colourimetry

I. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration
II. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
III. Study the kinetics of iodination of propanone in acidic medium.
IV. Determine the amount of iron present in a sample using 1,10-phenathroline.
V. Determine the dissociation constant of an indicator (phenolphthalein).
VI. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.
VII. Analysis of the given vibration-rotation spectrum of HCl(g)

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).

- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).

Semester VI

CHEMISTRY-C XIII: INORGANIC CHEMISTRY-IV (CBT-13)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Theoretical Principles in Qualitative Analysis (H_2S Scheme)

Basic principles involved in analysis of cations and anions and solubility products, common ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group II.

Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type.
Concept of hapticity of organic ligands.
Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Reaction Kinetics and Mechanism

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans-effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes.

Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinsons Catalyst)
2. Hydroformylation (Co salts)
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Synthesis gas by metal carbonyl complexes

Reference Books:

Recommended Texts:

- Vogel, A.I. *Qualitative Inorganic Analysis*, Longman, 1972

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall, 1996-03-07.
- Cotton, F.A. G.; Wilkinson & Gaus, P.L. *Basic Inorganic Chemistry 3rd Ed.;* Wiley India,
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed.,* Harper Collins 1993, Pearson,2006.
- Sharpe, A.G. *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005
- Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry3rd Ed.,* John Wiley and Sons, NY, 1994.
- Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements, Elsevier 2nd Ed,* 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
- Lee, J.D. *Concise Inorganic Chemistry 5th Ed.,* John Wiley and sons 2008.
- Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.
- Shriver, D.D. & P. Atkins, *Inorganic Chemistry 2nd Ed.,* Oxford University Press, 1994.
- Basolo, F. & Person, R. *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2nd Ed.,* John Wiley & Sons Inc; NY.
- Purcell, K.F. & Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977
- Miessler, G. L. & Donald, A. Tarr, *Inorganic Chemistry 4th Ed.,* Pearson, 2010.
- Collman, James P. et al. *Principles and Applications of Organotransition Metal Chemistry*. Mill Valley, CA: University Science Books, 1987.
- Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals. j* New York, NY: John Wiley, 2000.
- Spessard, Gary O., &Gary L. Miessler. *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

CHEMISTRY PRACTICAL-C XIII INORGANIC CHEMISTRY-IV (CBL-13)

LAB 60 Lectures

Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, CH_3COO^-, F^-, Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}

Mixtures should preferably contain one interfering anion, **or** insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3)**or** combination of anions e.g. CO_3^{2-} and SO_3^{2-}, NO_2^- and NO_3^-, Cl^- and Br^-, Cl^- and I^-, Br^- and I^-, NO_3^- and Br^-, NO_3^- and I^-.

Spot tests should be done whenever possible.

i. Measurement of 10 Dq by spectrophotometric method
ii. Verification of spectrochemical series.
iii. Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.
iv. Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complex.
v. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall, 1996-03-07.
- Cotton, F.A. G.; Wilkinson & Gaus, P.L. *Basic Inorganic Chemistry 3rd Ed.;* Wiley India,
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed.,* Harper Collins 1993, Pearson,2006.
- Sharpe, A.G. *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005
- Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry3rd Ed.,* John Wiley and Sons, NY, 1994.
- Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements, Elsevier 2nd Ed,* 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
- Lee, J.D. *Concise Inorganic Chemistry 5th Ed.,* John Wiley and sons 2008.
- Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.
- Shriver, D.D. & P. Atkins, *Inorganic Chemistry 2nd Ed.,* Oxford University Press, 1994.
- Basolo, F. & Person, R. *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2nd Ed.,* John Wiley & Sons Inc; NY.
- Purcell, K.F. & Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977
- Miessler, G. L. & Donald, A. Tarr, *Inorganic Chemistry 4th Ed.,* Pearson, 2010.
- Collman, James P. et al. *Principles and Applications of Organotransition Metal Chemistry*. Mill Valley, CA: University Science Books, 1987.
- Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals. j* New York, NY: John Wiley, 2000.
- Spessard, Gary O., &Gary L. Miessler. *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

CHEMISTRY PRACTICAL-C XIII INORGANIC CHEMISTRY-IV (CBL-13)

LAB 60 Lectures

Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, CH_3COO^-, F^-, Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}

Mixtures should preferably contain one interfering anion, **or** insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3)**or** combination of anions e.g. CO_3^{2-} and SO_3^{2-}, NO_2^- and NO_3^-, Cl^- and Br^-, Cl^- and I^-, Br^- and I^-, NO_3^- and Br^-, NO_3^- and I^-.

Spot tests should be done whenever possible.

i. Measurement of 10 Dq by spectrophotometric method
ii. Verification of spectrochemical series.
iii. Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.
iv. Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complex.
v. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Reference Books

- Vogel's *Qualitative Inorganic Analysis*, Revised by G. Svehla.
- Marr & Rockett *Inorganic Preparations*.

CHEMISTRY-C XI: ORGANIC CHEMISTRY-V (CBT-14)

(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

Carbohydrates:

Introduction, monosaccharadies, glycoside bond formation, mutarotation. Reactions of aldoses and ketoses (oxidation and reductions). Killiani synthesis, Osazone formation. Glucose-structure (including cyclic structure), Fructose (reactions only). Degradation of monosaccharaides: Ruff degradation.

Heterocyclic Compounds: Synthesis and chemistry of furan, thiophene, pyrrole, indole, pyridines, isoquinoline and quinoline.

Chemistry of Natural Products:
A study of the following compounds involving their isolation, structure elucidation and synthesis: Alkaloids- Hofmann exhaustive methylation, nicotine; Terpenes- Isoprene rule, citral.

Organic Synthesis *via* enolates: Preparation of DEM and EAA. Synthesis of mono/dicarboxylic acid, diketones, uracil, barbutric acid using DEM/EAA: Mukhayama Aldol reactions and Michael reactions.

Photochemistry: Principles of photochemistry, photochemical reactions of carbonyl compounds and olefins.

^{1}H NMR Spectroscopy: NMR phenomenon, precessional motion, Chemical shift, Shielding and de-shielding effects, Spin-spin splitting, Coupling constant, Interpretation of NMR spectra.

Books Recommended

1. "*Chemical Applications of Group Theory*" F. Albert Cotton, 3'rd Edition 1993, Wiley-India .
2. "*Environmental Chemistry*", A. K. De, 3rd Edition (1994), Wiley Eastern, New Delhi.
3. "*Analytical Chemistry*", G. D. Christian, 4th Edition (1986), John Wiley & Sons, New York.
4. "*Principles of Instrumental Analysis*", D.A. Skoog, 5th Edition (1998), Saunders College Publishing, Philadelphia, London.y, New York.
5. "*Basic Concepts of Analytical Chemistry*", S. M. Khopkar, 2nd Edition (1998), New Age International Publications, New Delhi.
6. "*Instrumental Methods of Analysis*", H. H. Willard, L. L. Merritt, and J. A. Dean, 6th Edition (1986),CBS Publishers & Distributors, Shahdara, Delhi.
7. "*Organic Chemistry*", I. L. Finar, [Vol. 2, 6th Edition (1973), Reprinted in 1980 & Vol. II, 5th Edition (1975), Reprinted in1996], ELBS and Longman Ltd., New Delhi.

CHEMISTRY PRACTICAL-C XI : ORGANIC CHEMISTRY-V LAB (CBL-14)

60 Lectures

1. Preparation of organic dyes.
2. Preparation of organic compounds

Reference Books:

1. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry 5th Ed., Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
4. Ahluwalia, V.K. &Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

CHEMISTRY-DSE I-IV (ELECTIVES)

CHEMISTRY-DSE-I: ANALYTICAL METHODS IN CHEMISTRY

(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

(5 Lectures)
Optical methods of analysis:

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;

Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

Structural illustration through interpretation of data, Effect and importance of isotope substitution.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

Thermal methods of analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation, Techniques for quantitative estimation of Ca and Mg from their mixture.

Electroanalytical methods:

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pK_a values.

Separation techniques:

Solvent extraction: Classification, principle and efficiency of the technique.

Mechanism of extraction: extraction by solvation and chelation.

Technique of extraction: batch, continuous and counter current extractions.

Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

Chromatography: Classification, principle and efficiency of the technique.

Mechanism of separation: adsorption, partition & ion exchange.

Development of chromatograms: frontal, elution and displacement methods.

Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).

Role of computers in instrumental methods of analysis.

Reference Books:

- Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore.
- Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
- Ditts, R.V. Analytical Chemistry – Methods of separation.

PRACTICALS- DSE-I LAB: ANALYTICAL METHODS IN CHEMISTRY

60 Lectures

I. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Fe^{3+}, Al^{3+}, and Cr^{3+}.

(ii) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R_f values.

(b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their R_f values.

(c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

II. Solvent Extractions:

(i) To separate a mixture of Ni^{2+} & Fe^{2+} by complexation with DMG and extracting the Ni^{2+}-DMG complex in chloroform, and determine its concentration by spectrophotometry.

(ii) Solvent extraction of zisconium with amberliti LA-1, separation from a mixture of irons and gallium.

3. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.

4. Determination of Na, Ca, Li in cola drinks and fruit juices using fame photometric techniques.

5. Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium, phosphate, nitrate

6. Ion exchange:

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.

(ii) Separation of metal ions from their binary mixture.

(iii) Separation of amino acids from organic acids by ion exchange chromatography.

III Spectrophotometry

1. Determination of pK_a values of indicator using spectrophotometry.
2. Structural characterization of compounds by infrared spectroscopy.
3. Determination of dissolved oxygen in water.
4. Determination of chemical oxygen demand (COD).
5. Determination of Biological oxygen demand (BOD).
6. Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by Job's method.

Reference Books:

- Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore.
- Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.

CHEMISTRY-DSE-II: BIOCHEMSITRY

Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Amino acids: Amino acids – Preparative methods, physical properties, dipolar nature, chemical reactions and configuration. Concept of unnatural amino acids. Importance of amino acids.

Peptides and Proteins: Peptides: Peptide-linkage, peptide synthesis and structure of polypeptides. Proteins: General characteristics and primary, secondary and tertiary structure. Common deficiency diseases.

Metalloproteins: Enzymes: Classification, nomenclature, co-enzymes (representative examples from different classes). Enzyme kinetics and enzyme inhibition. Hemoglobin: Oxygen and carbon dioxide transport by hemoglobin.

Vitamins and Hormones: Chemical constitution and physiological functions of vitamins A, B2 (Riboflavin), C (Ascorbic acid); Thyroxin and estrone.

Drugs: Classification, preparation and Mechanism of action of the following:
(i) Antipyretics and Analgesics : Aspirin, Paracetamol,
(ii) Sulpha drugs: Sulphanilamide, Sulphaguanidine
(iii)Antimalarials: Chloroquine
(iv) Antibiotics: Chloramphenicol.

Books Recommended

1. *"Organic Chemistry"*, **R. T. Morrison and R. N. Boyd**, 6th Edition (1992), Prentice-Hall of India (P) Ltd., New Delhi.
2. *"Organic Chemistry"*, **S. M. Mukherji , S. P. Singh, and R. P. Kapoor**, 1st Edition (1985), 5th Reprint (1999), New Age International (P) Ltd.Publishers, New Delhi.
3. *"Organic Chemistry"*, **I. L. Finar,** Vol. II, 5th Edition (1975), Reprinted in1996, ELBS and Longman Ltd., New Delhi.
4. "Biochemistry" **L. Stryer**, 5th edition (2002) Freeman & Co New York.

5. "Principles of Biochemistry" **D. L. Nelson M.M. Cox, Lehninger**, 3rd edition (2002) McMillan North Publication.

PRACTICALS- DSE-II LAB-I: BIOCHEMISTRY CHEMISTRY LAB

Identification and estimation of the following:

1. Carbohydrates – qualitative and quantitative.
2. Lipids – qualitative.
3. Proteins – qualitative.
4. Isolation of protein.
5. Determination of protein by the Biuret reaction.

Reference Books:

1. T.G. Cooper: Tool of Biochemistry.
2. Keith Wilson and John Walker: Practical Biochemistry.
3. Alan H Gowenlock: Varley's Practical Clinical Biochemistry.
4. Thomas M. Devlin: Textbook of Biochemistry.
5. Jeremy M. Berg, John L Tymoczko, Lubert Stryer: Biochemistry.
6. G. P. Talwar and M Srivastava: Textbook of Biochemistry and Human Biology.
7. A.L. Lehninger: Biochemistry.O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods
5. Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, for e.g. salicylic acid, cinnamic acid, nitrophenols etc.
6. Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).

CHEMISTRY-DSE-III: NOVEL INORGANIC SOLIDS

Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Synthesis and modification of inorganic solids:
Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

Inorganic solids of technological importance:
Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments. Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

Nanomaterials:
Overview of nanostructures and nanomaterials: classification. Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and antisical nanomaterials, bionano composites.

Asymmetric Catalysis on Industrial Scale

Overview on asymmetric catalysis, Asymmetric Hydrogenations – The Monsanto L-Dopa Process, Biocatalytic Approaches for the Large-Scale Production of Asymmetric Synthons, Methods for the Enantioselective Biocatalytic Production of L-Amino Acids on an Industrial Scale, Industrialization Studies of the Jacobsen Hydrolytic Kinetic Resolution of Epichlorohydrin.

Micro and mesoporous materials
Introduction, Zeolites and MCM-41/48 preparation, properties ,composition and structure and structural characterization. Functionalizations and applications as solid support and heterogeneous catalyst, shape selective catalysis.

Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene and polypyrole, applications of conducting polymers, Ion-exchange resins and their applications. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

Reference Books:

• Shriver & Atkins. *Inorganic Chemistry*, Peter Alkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, 5th Edition, Oxford University Press (2011-2012)
• Adam, D.M. *Inorganic Solids: An introduction to concepts in solid-state structural chemistry.*
• Frank J. Ovens, *Introduction to Nanotechnology*
• Blaser Hans-Ulrich, Schmidt Elke (Editors) *Asymmetric Catalysis on Industrial Scale: Challenges, Approaches and Solutions* (2004) ISBN:9783527602155

CHEMISTRY PRACTICAL - DSE LAB-III: NOVEL INORGANIC SOLIDS

60 Lectures

1. Study of optical activity of chiral molecules
2. Synthesis of polymers: like Nylon (6,6)
3. Synthesis of hydrogel by co-precipitation method.
4. Synthesis of metal/metal oxide nanoparticles.

Reference Book:

• Fahan, *Materials Chemistry,* Springer (2004).

CHEMISTRY-DSE-IV: POLYMER CHEMISTRY

(Credits: Theory-06, Practicals-02)
Theory: 60 Lectures

Introduction and history of polymeric materials:

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

Functionality and its importance:

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bi-functional systems, Poly-functional systems.

Kinetics of Polymerization:

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

Crystallization and crystallinity:

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

Nature and structure of polymers-Structure Property relationships.

Determination of molecular weight of polymers (M_n, M_w, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance.

Polydispersity index.

Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg).

Polymer Solution – Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory-Huggins theory, Lower and Upper critical solution temperatures.

Properties of Polymers (Physical, thermal, Flow & Mechanical Properties).

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes,

Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

Reference Books:

- *Seymour's Polymer Chemistry,* Marcel Dekker, Inc.
- G. Odian: Principles of Polymerization, John Wiley.
- F.W. Billmeyer: Text Book of Polymer Science, John Wiley.
- P. Ghosh: Polymer Science & Technology, Tata Mcgraw-Hill.
- R.W. Lenz: Organic Chemistry of Synthetic High Polymers.

CHEMISTRY PRACTICAL - DSE LAB: POLYMER CHEMISTRY

60 Lectures

1. Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
    a. Purification of monomer
    b. Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutylonitrile (AIBN)
2. Preparation of nylon 66/6

1. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
    a. Preparation of IPC
    b. Purification of IPC
    c. Interfacial polymerization
3. Redox polymerization of acrylamide
4. Precipitation polymerization of acrylonitrile
5. Preparation of urea-formaldehyde resin
6. Preparations of novalac resin/resold resin.
7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight by viscometry:
    (a) Polyacrylamide-aq.$NaNO_2$ solution
    (b) (Poly vinyl proplylidine (PVP) in water
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
2. Instrumental Techniques
3. IR studies of polymers
4. DSC analysis of polymers
5. Preparation of polyacrylamide and its electrophoresis

Reference Books:

- Malcohm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
- Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
- Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
- Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)

- Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
- L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)
- Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

CHEMISTRY-DSE-V: APPLICATIONS OF COMPUTERS IN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Basics:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

Numerical methods:

Roots of equations: Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.

Differential calculus: Numerical differentiation.

Integral calculus: Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values.

Simultaneous equations: Matrix manipulation: addition, multiplication. Gauss-Siedal method.

Interpolation, extrapolation and curve fitting: Handling of experimental data.

Conceptual background of molecular modelling: Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

Reference Books:

- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.

- Noggle, J. H. *Physical chemistry on a Microcomputer.* Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style.* Jaico Publishing House: Delhi (1996).

PRACTICAL-DSE V LAB: APPLICATIONS OF COMPUTERS IN CHEMISTRY

60 Lectures

Computer programs based on numerical methods for:

1. Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid).
2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.

4. Matrix operations. Application of Gauss-Siedel method in colourimetry.
5. Simple exercises using molecular visualization software.

Reference Books:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical Chemistry on a Microcomputer*. Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style.* Jaico Publishing House: Delhi (1996).

CHEMISTRY-DSE-VI: RESEARCH METHODOLOGY FOR CHEMISTRY

(Credits: Theory-05, Tutorials-01)
Theory: 75 Lectures

Literature Survey:

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

Methods of Scientific Research and Writing Scientific Papers:

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism.

Chemical Safety and Ethical Handling of Chemicals:
Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

Data Analysis
The Investigative Approach: Making and Recording Measurements. SI Units and their use.Scientific method and design of experiments.

Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, *r* and its abuse. Basic aspects of multiple linear regression analysis.

Electronics
Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

Reference Books

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2nd Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
- Topping, J. (1984) *Errors of observation and their treatment.* Fourth Ed., Chapman Hall, London.
- Harris, D. C. *Quantitative chemical analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis.* Cambridge Univ. Press (2001) 487 pages.
- Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
- OSU safety manual 1.01.

CHEMISTRY-DSE-VII: GREEN CHEMISTRY

(Credits: Theory-04, Practicals-02)
Theory: 60 Lectures

Introduction to Green Chemistry
What is Green Chemistry? Importance of Green Chemistry. Goals of Green Chemistry. Limitations/Obstacles in the pursuit of the goals of Green Chemistry

Principles of Green Chemistry and Designing a Chemical synthesis
Twelve principles of Green Chemistry with their explanations and special emphasis on the following with examples:
(i) Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products , Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
(ii) Prevention/ minimization of hazardous/ toxic products reducing toxicity risk = (function) hazard x exposure ; waste or pollution prevention hierarchy
(iii) Green solvents– super critical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents
(iv) Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy
(v) Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups;
(vi) Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, bio catalysis, asymmetric catalysis and photo catalysis.
(vii) Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD —What you don't have cannot harm youl, greener alternative to Bhopal Gas Tragedy (safer route to carbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.
(viii) Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Examples of Green Synthesis/ Reactions and some real world cases

1. Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)
2. Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
3. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)
4. Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO2 for precision cleaning and dry cleaning of garments.
5. Designing of Environmentally safe marine antifoulant.
6. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
7. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.
8. Healthier Fats and oil by Green Chemistry: Enzymatic Inter esterification for production of no Trans-Fats and Oils
9. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis (C2S3); Green chemistry in sustainable development.

Reference Books:

1. Ahluwalia, V.K. and Kidwai, M.R. *New Trends in Green Chemistry*, Anamalaya publishers, 2005
2.Anastas, P.T. and Warner, J.K. *Oxford Green Chemistry -Theory and Practical*, University Press, 1998
3. Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker, 2001
4. Cann, M.C. and Connely, M.E. *Real-World Cases in Green Chemistry*, American Chemical Society, Washington, 2000
5. Ryan, M.A. and Tinnesand, M., *Introduction to Green Chemistry*, American Chemical Society Washington, 2002
6. Lancaster, Mike, *Green Chemistry an Introductory Text* 2nd Ed., RSC Publishing,. ISBN: 978-1-84755-873-2

CHEMISTRY PRACTICAL - DSE – VII LAB: GREEN CHEMISTRY

1. Safer starting materials

Preparation and characterization of nano particles of gold using tea leaves.

2. Using renewable resources

Preparation and characterization of biodiesel from vegetable oil/ waste cooking oil

3. Use of enzymes as catalysts

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide

4. Alternative sources of energy

Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).

5. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

Reference Books:

1. Anastas, P.T and Warner, J.C. *Green Chemistry: Theory and Practice,* Oxford University Press, 1998
2. Kirchoff, M. and Ryan, M.A. *Greener approaches to undergraduate chemistry experiment.* American Chemical Society, Washington DC, 2002
3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC, 2002
4. Sharma, R.K.; Sidhwani, I.T. and Chaudhari, M.K. *Green Chemistry Experiments: A monograph,* I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7, 2013
5. Cann, M.C. and Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society, 2008
6. Cann, M. C. and Thomas, P. *Real world cases in Green Chemistry,* American Chemical Society, 2008
7. Lancaster, Mike *Green Chemistry: An introductory text*: 2nd Ed. RSC publishing, ISBN 978-1-84755-873-2
8. Pavia, D.L., Kriz, G.S., Lampman, G.M. and Engels, R.G. *Introduction to Organic Laboratory Techniques – a Microscale Approach* 4th Ed., Brooks-Cole Laboratory Series for Organic Chemistry, 2006

CHEMISTRY-DSE-VIII- DISSERTATION/ PROJECT WORK FOLLOWED BY SEMINAR (DSC-IV-Project)