M.Sc. Programme in CHEMISTRY

Course Structure, Syllabus

Department of Chemistry

School of Chemical Sciences

Central University of Karnataka

Programmed Offered & Intake

Programmes	Duration	Intake	Extranumerary			
M.Sc.	4 Semesters	30	03 (HKR)	01 (NSS/NCC/Sports)	01 (WDP)	01 (PWD)
Ph.D.	8 -12 semester	As per the available vacancy in the Department				

Some of the facility available in the Department:

- Class rooms with Green Board, White Board & Wi-Fi facility
- Projector for power point presentation
- State of art Laboratory with 56 work benches
- Laboratory feature include safety measures like eye wash, shower, fume hood with exhaust & CO_2 fire extinguisher
- UV-Visible spectrometer
- FT-IR spectrometer
- Gas chromatography
- Electrochemical work station
- Rotary evaporators (03 Nos.)
- Ice-Flakes Machine
- Equipped with other minor equipments like Air oven, water bath, pH meter, centrifuge machine, conductivity meter, potentiometer, refrigerator, heating mantles, magnetic stirrers etc.

M.Sc. Chemistry
Course Structure (CBCS Pattern)
Central University of Karnataka, Gulbarga.

Semester-I **No. of credits = 22**

Code	Type	Title	Credits	Hours
CY-401	Core-1	Inorganic Chemistry – I	4	4
CY-402	Core-2	Organic Chemistry – I	4	4
CY-403	Core-3	Physical Chemistry – I	4	4
CY-404	Soft Core-1	Introduction to Analytical Chemistry	3	3
CYL-405	SEC-1	Inorganic Chemistry Laboratory	2	4
CYL-406	SEC-2	Organic Chemistry Laboratory	2	4
	Open Elective		3	3
Total			22	26

Semester-II **No. of credits = 19**

Code	Type	Title	Credits	Hours
CY-407	Core-4	Inorganic Chemistry – II	4	4
CY-408	Core-5	Organic Chemistry – II	4	4
CY-409	Core-6	Physical Chemistry – II	4	4
CY-410	Soft Core-2	Chemistry of Life	3	3
CYL-411	SEC-3	Physical Chemistry Laboratory	2	4
CYL-412	SEC-4	Analytical & Computational Chemistry Laboratory	2	4
Total			19	23

Semester-III **No. of credits = 19**

Code	Type	Title	Credits	Hours
CY-501	Core-7	Group theory &Molecular Spectroscopy	4	4
CY-502	Core-8	Organometallics	3	3
CY-503	Core-9	Organic Chemistry-III	3	3
CY-504	Core-10	Spectroscopic Identification of Organic Compounds	4	4
CY-505	DSE-1	Elective-I	3	3
CYL-506	SEC-5	Advanced Chemistry laboratory	2	4
Total			19	21

Semester-IV **No. of credits = 22**

Code	Type	Title	Credits	Hours
CY-507	DSE-2	Elective-II	3	3
CY-508	DSE-3	Elective-III	3	3
CY-509	FC-1	Elective Foundation	2	2
CYP-510	SEC-6	Research Project & Comprehensive viva	12	18
CY-511	FC-2	Seminar (Compulsory foundation course)	2	2
Total			22	28

Total No. of Credits = 82

SEC-Skill Enhancement Course; DSE-Discipline Specific Elective; FC-Foundation Course

M.Sc. Chemistry
Course Content/Syllabus
Central University of Karnataka, Gulbarga.

Semester-I

CY 401: Inorganic Chemistry-I **Credit 4**

UNIT I-Atomic Structure and Periodic Table: Atom as nucleus with orbital electrons, concept of wave-functions, quantum numbers, Arrangement of elements inGroups in the Periodic Table, Different blocks of elements, periodic properties, atomic states and term symbols. Bonding and structure: Types of bonds, orbital symmetry and overlaps, concept of MO and VB theory, concept of hybridization, bond energy and covalent radii, conceptof resonance, molecular dipole moment; polarizing power and polarizability,Fajan's rules.

UNIT II-Inorganic Solids: Types of solids, covalent, ionic, molecular and metallic solids, lattice energy, cohesive energy and Medulong constants, Van der Waals forces,hydrogen bonding, unit cell, crystal lattices, structures. Imperfections in crystals (point defects and Fcenters).

UNIT III-P block elements, including noble gas compounds: Boron and Silicon based compounds: Boron hydrides (small boranes and their anions, B1−B4), boron nitride, borazines, carboranes, metalloboranes, metallocarboranes; silicates, silicones, diamond, graphite, zeolites. Nitrogen, Phosphorous, Sulphur and noble gas compounds: Hydrides, oxides and oxy acids of Nitrogen, Phosphorous, Sulphur and halogens; phosphazines, sulphur-nitrogen compounds, inter halogen compounds, pseudo halogens, noble gas compounds.

UNIT IV- Nuclear Chemistry& f-block elements: Nuclear chemistry: radioactive decay and equilibrium. nuclear reactions, Q value, cross sections, types of reactions, chemical effects of nuclear transformations; fission and fusion, fission products and fission yields; radioactive techniques, tracer technique. Chemistry of lanthanides and actinides: lanthanide contraction, oxidation states, spectral and magneticproperties, use oflanthanide compounds asshift reagents.

UNIT V-Clathrates, rings, cages and supramolecular chemistry: Poly anions and isopoly anions, heteropoly anions; clathrates (noble gases, phosphazines) hydrogen bonding in clathrates, Phosphorous and Oxygen cagecompounds. Supramolecular chemistry, definition, host-guest interaction, cation, anion & neutral molecule binding hosts, crown ethers, calixarenes, application of supramolecular chemistry; supramolecular chemistry in biology

Reference books:

1. J. E. Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper and Row, 3rd Edn, 1983.
2. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., Pergamon Press, 1989.
3. D. F. Shriver, P.W. Atkins, C. H. Langford, Inorganic Chemistry, 2nd Edn, ELBS, 1994.
4. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.
5. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, A comprehensive Text, John Wiley, 5th Edn, 1987.

CY 402: Organic Chemistry-I **Credit- 4**

Unit I- Reaction mechanism and intermediates: Kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, methods of determining mechanisms, isotopes effects, effect of structure on reactivity; resonance, inductive, steric effect. Intermediates in reaction**:**Generation, structure stability and formation of carbocation, carbanion, non-classical carbocations, free radicals.**(14 hr)**

Unit II- Stereochemistry: Elements of symmetry, chirality, Projection formulae, enantiomers, diasteroisomers, racemic mixture and their resolution, configurational notations of simple molecules, DL and RS configurational notations, methods of resolution, optical purity, stereospecific and stereoselective synthesis, Asymmetric synthesis, Optical activity in the absence of chiral carbon, conformational analysis of cyclic compounds, effect of conformation on the course of rate of reactions, effect of conformation on reactivity, geometrical isomerism. **(20 hr)**

Unit III- Substitution reactions: The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanism, S_Ni mechanism, SE2 and SE1 mechanism. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium; ambident nucleophile, regioselectivity,S_NAr, benzyne and S_N1 mechanism.Arenium ion mechanism, ipso attack, orientation in other ring systems; Neighbouring group participation**(12 hr)**

Unit IV- Elimination and addition reactions: The E2, E1 and E1cB mechanisms, Hoffman and Saytzeff modes of elimination, orientation of the double bond, reactivity effects of substrate structures, attacking base, the leaving group and the medium, pyrolytic elimination. Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles, Regio- and chemoselectivity, orientation and reactivity.Reactivity of carbonyl group, nucleophilic addition of hetero-atoms (N,O), conjugate addition reactions.**(16 hr)**

Reference books:

1. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
2. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
3. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
4. Smith, M. B., March J., (Latest Ed.) *March's Advanced Organic Chemistry*, John Wiley and Sons, 6th edition, New York.
5. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition.
6. Eliel, E. L.; Wilen, S. H.(2008) *Stereochemistry of carbon compounds*. Wiley, Student edition.
7. Clayden, J.; Greeves, N.; Warren, S., (2012)*Organic Chemistry*, Oxford University press, 2nd edition.
8. Bruice Paula, Y., (2015). *Organic Chemistry*, 7th Edition, Pearson Edition.
9. Nasipuri, Stereochemistry of Organic Compounds.

CY 403: Physical Chemistry-I Credit - 4

UNIT I-Equilibrium Thermodynamics: Concept of workand heat, first law of thermodynamics, enthalpy and heat capacities- concept of entropy, second law of thermodynamics, third law of thermodynamics-residual entropy. Free energy, chemical potential, fugacity, liquids and solutions: ideal and non-ideal solutions, chemical equilibrium. [15 hrs]

UNIT II-Statistical Thermodynamics:BE, FD, MB statistics and distribution, ensembles, partition functions and molecular partition functions, mean energy, Residual entropy, heat capacity of monoand diatomic gases, chemical equilibrium, Einstein and Debye theories of heat capacity ofsolids. Non-equilibrium thermodynamics, Postulates and methodologies, linear laws, Gibbs equation, Onsager reciprocal theory. [15 hrs]

UNIT III-Quantum Chemistry I: Introduction, Classical mechanics, Lagrange & Hamiltonian equation, Inadequacy & need for quantum mechanics, postulates, operators & operator algebra, eigen values, eigen vectors& commutation relation. [15 hrs]

UNIT IV-Quantum Chemistry II: WaveMechanics Solution of Schrödinger's equation, particle in 1D, 2D & 3D boxes, Electron spin & Zeeman effect, variation & perturbation methods, Hartree and Hartree-Fock self consistent field model, Electronic configuration of atoms, addition of angular momenta, spectroscopic term symbols, spin-orbit coupling, selection rules for atomic spectra, Electronic configuration of atoms, addition of angular momenta, spectroscopic term symbols, selection rules for atomic spectra. [15 hrs]

Reference books:

1. P. W. Atkins, Physical Chemistry, 9thEdtion Oxford University Press, 2010.
2. L.A. Woodward, Molecular Statistics, Oxford University Press.
3. Y. V.C. Rao, An Introduction to Thermodynamics, Wiley Eastern, 1993.
4. Physical Chemistry, R.S.Berry, S.A.Rice and J.Ross, Oxford, 2001.
5. M. Ladd, Introduction to Physical Chemistry, Cambridge, 1998.
6. J. Rajaram & J.C. Kuriacose, Chemical Thermodynamics: Classical, Statistical and Irreversible. Pearson, 2013
7. D. A. McQuarrie and J. D. Simon Physical Chemistry, A molecular Approach, Viva, 1998.
8. F. W. Sears & G. L. Salinger, Thermodynamics, Kinetic Theory & Statistical Thermodynamics, Narosa, 1986.
9. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford, 1982.

CY 404: Introduction to Analytical Chemistry Credit -3

UNIT I: Thermal Analysis: Thermogravimetry (TGA), Differential Thermal Analysis (DTA), and Differential Scanning Calorimetry (DSC): definition, theoretical basis, instrumentation, factors affecting the data curve, applications, advantages and disadvantages.

UNIT II: Errors analysis: Accuracy and precision, absolute, relative, determinate and indeterminate errors, statistical treatment of random errors, computation rules for significant figures, method of least squares, mean deviations, and standard deviation.

UNIT III: Titrations: Acid-base, complexometric, conductometric and potentiometric titration- theory of acid base indicators, Mohr, Volhard and Fajans methods , EDTA based titration, Redox indicators, and their use in volumetric analysis, iodometry and iodimetry.

UNIT IV: Separation Techniques: Solvent extraction, thin-layer chromatography, gas chromatography (GC), liquid chromatography (LC), high performance liquid chromatography (HPLC), ion exchange chromatography, gel permeation chromatography. Chromatography coupled instrumentation.

Reference books:

1. Douglas A. Skoog, Donald M. West, F. James Holler and Stanley R. Crouch, (2013).*Fundamentals of Analytical Chemistry*, 9th Edition,Cengage Learning.
2. James W. Robinson, Eileen M. Skelly Frame, George M. Frame II, (2005).*Undergraduate Instrumental Analysis*, Sixth Edition, Marcel Dekker, New York.
3. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, (2009).*Introduction to Spectroscopy*, Fourth Edition, Brooks/Cole Thomson Learning.
4. Gary D. Christian, Purnendu Das gupta, Kevin Schug, (2013). *Analytical Chemistry,* 7th Edition, Wiley.

CYL 405: Inorganic Chemistry Laboratory Credit -2

1) **Quantitative methods of Analysis**

1.1) Redox titrations

1.2) Complexometric titrations

1.3) Potentiometry: Ferrous ammonium sulphate (FAS) vs $KMNO_4$; Estimation of Mn^{2+} ion in Pyrolusite ore

1.4) Alloy analysis: Manganese in Steel by spectrophotometry

1.5) Acid Strength in a citrus fruit: pH titration method and also by conductometric analysis

2) **Inorganic complex Synthesis & analysis:**

2.1) Nickel complexes; Preparation of $[Ni(en)_3]S_2O_3$, $[Ni(H_2O)_6]Cl_2$, $[Ni(NH_3)_6]Cl_2$ and studying respective absorption spectra.

Reference books:

1. Text book of Quantitative Analysis, A.I. Vogel 4^{th}edn (1992)
2. Electronic Spectroscopy by A.B. P. Lever.
3. Inorganic Synthesis (Vol. Series)

CYL 406: Organic Chemistry Laboratory Credit-2

1. **Distillation techniques:** Fractional distillation, vacuum distillation etc. Purification and drying of common organic solvent.
2. **Organic Synthesis:** Single step synthesis of organic compounds. Aspects such as conversion, yield, selectivity, atom economy, economic factor, green protocol and safety practices should be paid attention.
    I. Synthesis of a chalcones via Claisen-Schmidt condensation
    II. Synthesis of dibenzalpropanone by Aldol condensation.
    III. Nitration of Salicylic acid by green approach.
    IV. Thin layer chromatography-understanding theory by determining $R_f$values for some common amino acids.
    V. Extraction of Chlorophyll pigment from Spinach leaves.
    VI. Preparation Aspirin by acetylation.
    VII. Synthesis of five membered heterocycle by cycloaddition method
    VIII. Preparation of allylic alcohols via Baylis-Hillman reaction using DABCO as a catalyst
    IX. Experiment for oxidation and reduction by using oxidizing and reducing agents.

The products are to be separated either by column chromatography or by recrystallization. The products are to be characterized by melting point, IR spectroscopy etc. Any 6-8 experiments will be conducted. Experiments should be added and altered according to availability in laboratory.

Reference books:

1. Vogel, A.I. (1996). *Text book of practical organic chemistry*, Pearson, 5th edition, UK.
2. Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan Limited, London.
3. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson, 4th edition, UK.
4. Pasto, D.P., Johnson, C., Miller, M. (1992). *Experiments and Techniques in Organic Chemistry*, Prentice Hall, 1st edition, US.
5. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
6. Williamson, K.L., Health, D.C. (1999). *Macroscale and Microscale Organic Experiments*, *Heath, D.C.* and Co., Lexington, MA.

Semester-II

CY 407: Inorganic Chemistry-II **Credit -4**

UNIT I-Introduction to transition metal complexes: Brief review ofthe general characteristics of transition elements, types of ligands, nomenclatureof coordination complexes, chelates, chelate effect, geometry and isomerism, formation of complexes, stability constants, Werner, Sidzwickand VSEPR theory.

UNIT II-Electronic structure of transition metal complexes 1: Crystal field theory, crystalfield splitting, application of d-orbital splitting to explain magnetic properties, low spin and high spin complexes, crystal field stabilization energy, spectrochemical series, weak and strongfield complexes, thermodynamicand related aspects of crystal fields, ionic radii, heats of ligation, lattice energies, site preferenceenergies.

UNIT III-Electronic structure of transition metal complexes 2:VB and MO theory of complexes (quantitative principles involved in complexes with no pi and with pi bonding) and ligand filed theoriesand molecular symmetry, angular overlap model, Jahn Teller effect, electronic spectra of transition metal complexes, Orgal and Tanabe-Sugano diagrams, charge transfer and d-d transitions, nephelauxetic series.

UNIT IV-Inorganic reaction mechanisms: Inert and labile compounds, substitution reactions of octahedral complexes, dissociative, associative, anation,aquation, conjugate base mechanism; substitution reactions of square planar complexes,transeffect, trans effect series, theories of trans effect; electron transfer reactions.

UNIT V-Magnetism: Dia, para, ferro and antiferromagnetism, quenching of orbital angular moment, spin orbit coupling.

Reference books:

1. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.
2. J. E. Huheey, Inorganic Chemistry, 3rd Edn., Harper International, 1983.
3. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rdEdn., John Wiley, 2001.
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.
5. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements,2nd Edn., BH, 1997.
6. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.

CY 408: Organic Chemistry-II Credit- 4

Unit I-Oxidations and reductions in organic synthesis: Mechanism, selectivity, stereochemistry and applications of selenium dioxide, Cr and Mn reagents, periodic acid, Osmium tetroxide, Swern oxidations, Baeyer-Villiger oxidation, ozonolysis, epoxidations using peracids. Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Wolff-Kishner reduction, Dissolving metal reductions, metal hydride reductions using $NaBH_4$, $LiAlH_4$, DIBAL, K-selectride, Sodium cyanoborohydride. **[15 hrs]**

Unit II-Reagents in organic synthesis: Lithiumdiisopropylamide(LDA), DicyclohexylCarbodiimide(DCC), Trimethylsilyliodide, Gilman's reagent, DDQ,Prevost Hydroxylation, Phase transfer catalysts, Phosphorous and Sulphurylides,Merifield resin, Lawson reagents, IBX, Ceric ammonium nitrate, Tebbe reagent. **[15 hrs]**

Unit III-Named Reactions & Rearrangements in organic synthesis: Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzillic acid, Favorskii, Neber, Beckmann, Hofmann, Curtius, Schimidt rearrangements, Arndt-Eister syntheses, Mukaiyama aldol reaction, Mitsunobu reaction, Sharpless epoxidation, Shapiro reaction, Vilsmeier–Haack reaction, Baylis-Hillman reaction, Biginelli reaction. **[16 hrs]**

Unit IV-Pericyclic reactions: Thermal and photochemical pericyclic reactions, Conrotation and disrotation; Electrocyclic closure and opening in 4n and 4n+2 systems. Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions and examples. Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Diels-Alder reaction, Woodward-Hoffmann selection rules for cycloaddition reactions and examples. Mechanism by orbital symmetry correlation diagrams, Fukui Frontier Molecular Orbital (FMO) theory. Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Sigmatropic reactions: mechanism of sigmatropic reactions, Cope and Claisen rearrangements.

[18 hrs]

Reference books:

1. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
2. Jie Jack Li, (2009). *Name Reactions: A collection of Detailed Reaction Mechanism*, Publisher: Springer-verlag.
3. McMurry J., *Organic Chemistry***,** Asian Book Pvt. Ltd, 8th edition, New Delhi.
4. Smith, M. B., March J., (Latest Ed.) *March's Advanced Organic Chemistry*, John Wiley and Sons, 6th edition, New York.
5. Clayden, J.; Greeves, N.; Warren, S., (2012) *Organic Chemistry*, Oxford University press, 2nd edition.
6. Sankaraman, S. (2005).*Pericyclic reactions: Reactions, Applications and Theory*, Wiley-VCH.
7. Kurti, L., Czako, B. (2005). *Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier Publications.

CY 409: Physical Chemistry-II Credit -4

UNIT I-Kinetics-I: Basic Chemical Kinetics Molecularity, order and rate of reactions, Arrhenius theory - Complex reactions: reversible, pre-equilibrium, consecutive, chain and photochemical, oscillatory reactions, enzyme kinetics - Lindenmann's theory of uni-molecular reactions - laser flash photolysis, flow techniques and relaxationmethods. **[12 hrs]**

UNIT II-Kinetics-II: Molecular reaction dynamics collision and activated complex theory, comparison of results with Eyring and Arrhenius equations - reactive collisions, molecular beam experiments, introduction to potential energy surfaces: treatment of H_2 + H reaction – ionicreactions:salt effect. **[12 hrs]**

UNIT III-Surface Chemistry: Surface phenomena Growth and structure of surface, surfacedefects, kinetics of surface adsorption: Langmuir and BET isotherms. **[12 hrs]**

UNIT IV-Electrochemistry-I: Equilibrium electrochemistry Activities in electrolytic solutions, mean activity coefficient, Debye-Huckel treatment of dilute electrolyte solutions, originof electrode potential, half-cellpotential, electrochemical cell, Nernst equation, thermodynamics of electrochemical cell**. [12 hrs]**

UNIT V-Electrochemistry-II: Dynamicelectrochemistry Electrical double layer - electrode kinetics: rate of charge transfer, current density, Butler- Volmer equation - introduction to polarography, cyclic voltammetry - theory of corrosion and inhibition of corrosion. **[12 hrs]**

Reference books:

1. K. J. Laidler, Chemical Kinetics, 3rd Edn., HarperInternational, 1987.
2. G. D. Billing & K. V. Mikkelson, Molecular dynamics and chemical kinetics, JohnWiley, 1996.
3. J. I. Sheinfield, J. S. Francisco, W. L. Hasse, Chemical kinetics & dynamics, Prientice Hall, 1998.
4. A. J. Bard & L. R. Faulkner, Electrochemical Methods, Fundamental and Applications, JohnWiley, 1980.
5. Bockris & Reddy, Electrochemistry, Vol. 1& 2, Plenum, 1973
6. H. V. Keer, Solid State Chemistry, Wiley Eastern, 1993.
7. A. K. Cheetam & P. Day, Solid State Chemistry Techniques, Oxford, 1987.

CY 410: Chemistry of Life Credit -3

UNIT I: Bioinorganic chemistry: Occurrence of elements, specific ligands, and coordination sites in biomolecules. Transport and storage of K^+, Ca^{2+} and Iron. Role of haemoglobin and myoglobin in transport and storage of oxygen. Electron Transfer: Cytochromes, Fe-S Clusters and Copper-Blue proteins. Catalysis: Acid-Base Catalases (Zn, Mg and Fe enzymes), Peroxidases. Molybdenum and tungsten enzymes. Nitrogen cycle. Bio mineralization. Applications: Sensing and medicinal. **[12 hrs]**

UNIT II: Biophysical chemistry: Chemistry and biology of water. Chemical forces responsible for stability of biomolecules; hydrogen bonding; electrostatic interactions, hydrophobic interactions; stacking interactions; covalent bonding; thermodynamic principles-of Biosystems-coupled reactions and protein folding; enzymes, catalysis, and kinetics- Michaelis-Menten equation, and Lineweaver–Burk plot; enzyme inhibition and different types of enzyme inhibition. **[08 hrs]**

UNIT III: Bioorganic chemistry: Biopolymers-DNA, RNA and Proteins- structures of monomers, bonding, and hierarchy of structural organization. Chemical methods involved in sequencing of DNA and Proteins. Chemical and biochemical synthesis of DNA- Phosphoramidite method and replication. Chemical and biochemical synthesis of peptides/proteins- solution phase and solid phase peptide synthesis methods and ribosomal synthesis of proteins. Applications of PNAS. **[12 hrs]**

UNIT IV: Natural product chemistry: Chemistry of terpenes- general methods, classification and special isoprene rule. Characterization of terpenes- Citral, limonene, carotene. Biosynthesis of acyclic and monocyclic terpenes from acetyl CoA. **:** Chemistry of steroids-Structure of common steroids such as cholesterol and steroidal hormones. Chemical and biochemical synthesis of cholesterol. Chemical synthesis of hormones using cholesterol. Chemistry of alkaloids - structure determination and synthesis of nicotine, morphine, cocaine. **[16 hrs]**

Reference books:

1. W. Kaim.; Bioinorgnic Chemistry, 2nd Edition, John Wiley. 2013.
2. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.
3. C.R. Cantor & P.R. Schimmel, Biophysical Chemistry, W.H.Freeman& Company, 1980
4. David Van Vranken and Gregory A, Introduction to Bioorganic Chemistry and Chemical Biology. Garland Science (Taylor & Francis), 2012.
5. R.H. Thomson, Chemistry of Natural Products - Wiley, New York, 1996.
6. I.L. Finar, Advanced Organic Chemistry, Vol. 2 ELBS, New Delhi, 1975.
7. Bhat, S.V., Nagasampagi, B.A., Meenakshi, S. (2009). *Natural Product Chemistry & Applications*, Narosa Publishing House, New Delhi.

CYL 411: Physical Chemistry Laboratory Credit -2

Physical chemistry lab experiments involves the use of potentiometry, spectrophotometry, pHmetry, conductometry & colorimetry instrument analysis

1) Reaction Kinetics: Decomposition of Benzene diazonium chloride
2) Enzyme Catalysis using UV-Vis spectrophotometer
3) Determination of pKa of a weak organic acid or a base using UV-Vis spectrophotometry
4) Potentiometry: Estimation of thermodynamic functions from EMF data measurements
5) Determination of stability constant of silver ammonia complex by potentiometric method
6) Verification of Beer-Lambert law using gold/silver nanoparticles
7) Estimation of excess thermodynamic properties of binary liquid mixture from density & ultrasonic velocity measurements
8) Determination of critical micelle concentration (CMC) of a surfactant in water by surface tension measurements
9) Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal
10) Estimation of Free energy of Protein denaturation using the intrinsic fluorescence of the protein
11) Heat of solution by solubility measurements
12) Electrochemical Oxidation of L-Cystine to L-Cysteic acid

Out of above list any 6-8 experiments will be conducted.

Reference books:

1. A. Findary, T. A. Kitchner, Practical physical chemistry. (Longmans, Green and Co.)
2. J. M. Wilson, K. J. Newcombe, A. R. Denko, R. M. W. Richett, Experiments in Physical Chemistry, (Pergamon Press)

CYL 412: Analytical & Computational Chemistry Laboratory Credit -2

1. Role of computer software & programme in solving chemistry problems
2. Introduction to different structure, object drawing & solving software's, structural elucidation & reaction pathway prediction using analytical tools, different mathematical & analytical tools (Gaussian, MATLAB & Mathematica) will be introduced

Reference books:

1. A. Findary, T. A. Kitchner , Practical physical chemistry, (Longmans, Green and Co.)
2. J. M. Wilson, K. J. Newcombe, A. R. Denko, R. M. W. Richett, Experiments in Physical Chemistry, (Pergamon Press)
3. F. Jensen, Introduction to Computational Chemistry (John Wiley and Sons Ltd.)

Semester-III

CY 501: Group theory and Molecular Spectroscopy Credit -4

UNIT I-Group Theory: Introduction, Molecular Symmetry & point groups, Symmetry elements and operators, classes of symmetry operation, Symmetry classification ofmolecules.Matrixrepresentation of symmetry operations, representation of groups, character, reducible and irreducible representations Great Orthogonality theorem, Character tables, symmetry propertiesof Hamiltonian operator, Mutual exclusion principle.

UNIT II-Rotational, Vibrational & Electronic spectroscopy: Electromagnetic radiation, interaction of electromagnetic radiation with matter, quantum mechanical approach - transition probabilities: Einstein coefficients - pure vibrational and rotational spectra, selection rules, vibrational and rotational spectra of polyatomic molecules, normal modes, anharmonicity, selection rules - Raman effect: classical and quantum theory of Raman effect, rotational and vibrational Raman spectra.Franck-Condon principle, Transition moments, assignment of electronic transitions of N_2, H_2O and formaldehyde using group theory, solvent effect, ESCA, PES, AUGER techniques.

UNIT III-Introduction to NMR:-Origin of magnetic moments in matter, electronic and nuclear moments, interaction with magnetic field, Larmor equation - conditions for magnetic resonance absorption, relaxation times, line widths and line shapes, ring currents, diamagnetic anisotropy, spin-spin splitting, high resolution NMR spectra of simple molecules, first and second order treatment of AB systems - FT techniques.

UNIT IV-Other Resonance Spectroscopy Methods:-EPR, NQR and Mossbauer spectroscopic techniques - Electron spin resonance: g value, hyperfine structure, ESR of organic free radicals, ESR of solids, ESR of inorganic ions, ESR of simple free radicals in solutions – NQR. The principles of Mossbauer spectroscopy. Origin of isomer shifts, quadrupole splitting and h. f. s.

Reference books:

1. P. W. Atkins, Physical Chemistry, Oxford, London, 7th edition,2006.
2. D. L. Pavia, G. M. Lampman and G. S. Kriz, “Introduction to Spectroscopy” 2ndEdn, Saunders
3. C.N. Banwell, Fundamentals of Molecular Spectroscopy, 4th Edition Tata McGraw Hill, 2016.
4. A. Carrington and Machlachlon, Magnetic Resonance, Harper & Row, 1967.
5. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.
6. D. H. Williams and I. Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, 1998.
7. J. Micheal Hollas, Modern Spectroscopy, 4th Edition, wiley India Pvt Ltd, 2010
8. Harald Gunther, NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry, 2nd Edition, Wiley India Pvt Ltd, 2010
9. F. Albert Cotton, Chemical Applications of Group Theory, 3rd Edition. Wiley, 2008

CY 502: Organometallics Credit – 3

UNIT I- Organometallic Chemistry 1: Compounds with transition metal to carbon bonds: classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: range of compounds and structure, bonding, vibrational spectra, preparation, reactions; transition metal organometallics: squareplanar complexes,metal alkyls, metal alkylidenes and metal alkylidynes; Structure and bonding: metal-olefin bond and arenemetal bond.

UNIT II-Organometallic Chemistry 2: Compounds with ligands having extended pi systems: bis(cyclopentadienyl) compounds, cyclopentadienyl carbonyl compounds, bis(arene) compounds, arene carbonyl compounds; isolobal analogy, metal-metal bond, transition metal clusters; clusters and catalysis; hydride and dihydrogen complexes; fluxionality.

UNIT III-Organometallic Chemistry 3: Organometallic reactions and catalysis: oxidative addition, reductive elimination,insertion, hydride elimination, abstraction; olefin hydrogenation,hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation,olefin metathesis, Monsanto aceticacid synthesis, Fischer-Tropsch process, hydrosilylation.

UNIT IV-Organometallics in Organic Synthesis:π-Bonding of Pd and Rh with olefins applications in C-C bond formations, Wacker reaction, Heck reaction, Carbonylation, hydroformylation, olefin isomerism, arylation, aryl amination using Pd reagents,olefin metathesis, Stille coupling,Sonogashira reaction, Buchwald reaction and Pauson -Khand reaction.

Reference books:

1. P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn., ELBS, 1991.
2. J. E. Huheey, *Inorganic Chemistry,* 3rd Edn., Harper International, 1983.
3. M. F. Purcell, J.C. Kotz, *Inorganic Chemistry*, Saunder, 1977.
4. F. A. Cotton, G. Wilkinson, *Advanced Inorganic Chemistry*, 5th Edn., JohnWiley.
5. R. W. Hay, *Bio Inorganic Chemistry*, Ellis Horwood, 1987.
6. R. M. Roat-Malone, *Bio Inorganic Chemistry*, John Wiley, 2002.
7. Clayden,J.; Greeves,N.;Warren,S., (2012).*Organic Chemistry*, Oxford University press, 2nd edition.

CY 503: Organic Chemistry-III Credit – 3

UNIT I-Photochemistry: Franck-Condon principle, Jablonski diagram, fluorescence and phosphorescence, Singlet and triplet states, Photosensitization, Quantum efficiency, Photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Photochemistry of enones and para-benzoquinones, Di π – methane rearrangement, Photodynamic therapy, Photochemical [4+2] cycloaddition using singlet Oxygen; Barton reaction. **[16 hrs]**

UNIT II-Synthetic strategies & Green Chemistry: Synthon, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination. Criteria for selection of target; Linear and convergent synthesis; Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations; Criteria for disconnection of strategic bonds; One group and two group C-X disconnections in 1,2-, 1,3-, 1,4 difunctional compounds. Protection and deprotection of functional groups in synthetic strategy: Protection of alcohols by silyl ethers and ester formations and their deprotection; Protection of 1, 2 diols- by acetal, ketal and their deprotection; Protection of amines by *t*- butoxycarbonyl, fmoc, and their deprotection, Protection of carbonyls by acetal and ketal formation and their deprotection. Green Chemistry principles and atom economy. **[20 hrs]**

UNIT III- Thermodynamically and kinetically controlled reactions with carbonyl compounds, regionand stereo-selective reactions. Enolates: Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, Effect of solvent, Counter cation and Electrophiles; Symbiotic effect; Thermodynamically and kinetically controlled enolate formations; Various transition state models to explain steroselectiveenolate formation; Enamines; Regioselectivity in generation, Application in controlling the selectivity of alkylation. **[12 hrs]**

Reference books:

1. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products.* Dorling Kindersley Pvt. Ltd., 6th edition, India.
2. McMurry J., *Organic Chemistry***,** Asian Book Pvt. Ltd, 8th edition, New Delhi.
3. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
4. Clayden,J.;Greeves,N.;Warren,S., (2012). *Organic Chemistry*, Oxford University press, 2nd edition.
5. Warren S.; Wyatt, P. (2008). *Organic Synthesis The Disconnection Approach*, Wiley 2nd edition.
6. Coyle, J. D. (1991), *Introduction to organic photochemistry*, Wiley.
7. Halton, B.; Coxon J. M. (2011), *Organic Photochemistry*, Cambridge University Press.
8. Smith, M. B.; March, J. (2007), *March's Advanced Organic Chemistry*, Wiley 6th edition.

CY 504: Spectroscopic Identification of Organic Compounds Credit – 4

UNIT I: Introduction to spectroscopic techniques: Structure elucidation. Application of UV – Visible and IR spectroscopy to organic structure elucidation. Electromagnetic spectrum, absorption of energy by organic compounds, types of spectroscopic methods to organic structure elucidation. Woodward – Fisher rules, Octant rule, Application of ORD – CD to stereochemical assignments. Organic functional group identification through IR spectroscopy.

UNIT II: Application of NMR Spectroscopy. Basic principles. Introduction to NMR techniques. CW and FT NMR techniques. ^{1}H NMR Spectral parameters – intensity, chemical shift, multiplicity, coupling constant. Analysis of first order and second - order spectra. Structure determination of organic compounds by ^{1}H NMR spectra.

UNIT III: Multinuclear ^{1}H NMR& ^{13}C NMR: Proton coupled, off resonance decoupled, proton noise decoupled ^{13}C NMR spectra. Assignment of chemical shifts, additively effect, characteristic chemical shifts of common organic compounds and functional groups, DEPT & SEFT spectra. 2D NMR techniques ^{1}H – ^{1}H COSY, ^{1}H – ^{13}C COSY – HMBC, and NOESY.

UNIT IV: Application of mass spectrometry: Basic principles, mass analyzers, ionization methods: EI, PI, CI, FAB, MALDI, ES. Liquid chromatography and mass spectrometry, types of ions and fragmentations, even electron rule, nitrogen rule, isotope abundance, McLafferty rearrangement.
Organic structure elucidation, techniques of ion production, ion and daughter ions, molecular ion and isotope abundance. Nitrogen rule energetics of fragmentation, metastable ions, common fragmentation pathways, fragmentation pattern of common chemical classes. Illustrative examples from macromolecules and supramolecules.

Reference books:

1. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, 6thEdn, Wiley.
2. W. Kemp, Organic Spectroscopy, 3rdEdn.,MacMillon, 1994.
3. Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3rdEdn., Brooks/Cole.
4. D. H Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill,1998.
5. W. Kemp, Introduction to multinuclear NMR.
6. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2004.

CYL 506: Advanced Chemistry Laboratory Credit-2

1. Selected organic chemistry experiments comprising 2-4 steps synthesis.
   Ex. Synthesis of Propanolol.
   The products are to be separated either by column chromatography or by recrystallization. The products are to be characterized by melting point, IR spectroscopy etc.
2. Experiment demonstrating protection &deprotection of functional group, Experiment depicting Grignard reagent generation and its reaction.
3. Photochemistry experiment/Belousov–Zhabotinsky reaction.
4. Introduction to explosive chemistry and exposure to explosive chemistry.
5. Selected Inorganic chemistry experiments like preparation of metal complexes and characterization.
6. Isolation of carotene and its UV spectral confirmation.
7. Selected Physical and Material Chemistry experiments.
8. Structure interpretation from Spectra.

Reference books:

1. Vogel, A.I. (1996). *Text book of practical organic chemistry*, Pearson, 5th edition, UK.
2. Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmilan Limited, London.
3. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson, 4th edition, UK.
4. Pasto, D.P., Johnson, C., Miller, M. (1992). *Experiments and Techniques in Organic Chemistry*, Prentice Hall, 1st edition, US.
5. A. Findary, T. A. Kitchner, Practical physical chemistry, (Longmans, Green and Co.)
6. J. M. Wilson, K. J. Newcombe, A. R. Denko, R. M. W. Richett, Experiments in Physical Chemistry, (Pergamum Press).
7. Text book of Quantitative Analysis, A.I. Vogel 4thedn (1992).
8. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, 6thEdn, Wiley.
9. Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks/Cole.

Subjects Offered in Discipline Specific Electives
(CY 505 Elective-I, CY 507 Elective-II & CY 508 Elective- III)

1. Introduction to Nanoscience
2. Applied Electrochemistry
3. Heterocycles and Metallopharmaceuticals
4. Introduction to Medicinal Chemistry
5. Biological Chemistry
6. Proteomics in Mass Spectroscopy
7. Green Chemistry
8. Advanced Stereochemistry
9. Chemistry of Natural Products
10. Advanced Stereochemistry

Electives will be floated according to availability of expert faculty members in the Department. Students will be given choice to select and as per majority students choice elective will be conducted. In total three discipline specific electives students have to take for completing M.Sc. Course.

Open Elective:

Students have to take one Open elective course from other departments in the University, preferably of 3 credits. Students are encouraged to take the opportunity to learn other aligned or non-aligned subjects as Open elective. Students can choose the options to improve their language proficiency, IT proficiency, personality development etc.

Foundation Course-1: Elective Foundation

CY 509: Credit-2

As per the UGC guideline for CBCS, a value based Man Making Education Course is designed for M.Sc. Chemistry students. Out of following three courses, one of the course will be conducted as per the majority of student's choice and availability of the expert faculty.

1. **Intellectual Property Rights, Innovations & Entrepreneurship:**

Innovation: Successful Innovation has at least three components-an insightful idea, significant value for the user and delivery to the market. Innovation spans across finding the right opportunity, generating ideas, building innovative solutions, protecting the intellectual property around the new idea and overcoming the barriers to the market. The students will be exposed to a structured method of growing ideas into innovation. The students will be exposed to open innovation and other collaborative approaches.

Intellectual Property Laws: The students will then be trained on IP creation and management.

Entrepreneurships: the students will finally be trained to think like entrepreneurs, create a business case for their idea and take their idea successfully to the market.

Reference books:

1. Acharya, N. K., (2001). *Textbook on intellectual property rights,* Asia Law House.
2. Ganguli, P. (2001). *Intellectual Property Rights; Unleashing the Knowledge Economy*, Tata McGraw-Hill.
3. Watal Jayashree, *Intellectual Property Rights in the WTO and developing countries*, Oxford University Press, Oxford.
4. Guru Manjula, Rao, M.B., (2003). *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications.

2. **Laboratory Safety & Laboratory Management**

3. **Discoveries in Chemistry**

4. **Environmental Chemistry**

CYP 510: Research Project & Comprehensive viva **Credit-12**

Individual faculty members will float stipulated number of projects. Students have to consult respective faculty members and select projects. More than one student can work under a single project based on nature of the project. Guide allotment for MSc project will be based on choice cum merit.

Once guide allotment (either single or more than one guide) is declared, student has to submit research proposal and give a presentation, either individually or one member from the group. Research proposal & presentation carries 20% of the marks. Students will be periodically assessed for their project work by individual faculty member or group of faculty members and 20% of the marks will be credited for this continuous assessment.

The final submission of the research project i.e. small thesis, presentation and comprehensive viva carries 60% marks.

Note:

1. Student should submit 3 copies of the final research project copy in hard binding format with all declarations and signatures.
2. For referencing any ACS journal pattern should be followed.

Foundation Course-2: (Compulsory Foundation)

As per the UGC guideline for CBCS, a Compulsory Foundation Course is designed for M.Sc. Chemistry students. Students have to give Seminar on recent research literature. The course will enhance the student's ability to present a subject, understand the relevant scientific literature, enhance stage courage and improve the ability to think or ponder over a research topic.

CY 511: Seminar **Credit-2**

Student should approach faculty members for seminar presentation on recent literature on particular topic.