Syllabus

for

Five Year Integrated Bachelor and Master of Science Programme

Department of Applied Chemistry

Cochin University of Science and Technology

(with effect from 2018-2019)

SEMESTER – I

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
ENG 10101	English – I	C	50	50	100	2
MAL 10101/ HIN 10101	Malayalam – I /Hindi – I	C	50	50	100	2
CHE 10101	Atomic Structure and Chemical Bonding	C	50	50	100	3
PHY 10101	Mechanics	C	50	50	100	3
MAT 10101	Calculus I	C	50	50	100	4
BIO 10101	Biology – I	C	50	50	100	3
CHE 10102	Chemistry Lab – Quantitative Analysis I	C	100	-	100	2
PHY 10102	Physics Lab – Mechanics	C	100	-	100	2
BIO 10102	Biology Lab – I	C	100	-	100	2
	Total		600	300	900	23

SEMESTER – II

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
ENG 10201	English – II	C	50	50	100	2
MAL 10201/ HIN 10201	Malayalam – II/ Hindi – II	C	50	50	100	2
CHE 10201	Periodicity, Nuclear Chemistry, Acid Base Chemistry and Metallurgy	C	50	50	100	3
PHY 10201	Waves and Optics	C	50	50	100	3
MAT 10201	Linear Algebra, Group Theory	C	50	50	100	4
BIO 10201	Biology – II	C	50	50	100	3
CHE 10202	Chemistry Lab – Qualitative Analysis I	C	100	-	100	2
PHY 10202	Physics Lab – Waves and Optics	C	100	-	100	2
BIO 10202	Biology Lab – II	C	100	-	100	2
	Total		600	300	900	23

SEMESTER – III

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 10301	Introductory Organic Chemistry	C	50	50	100	3
PHY 10301	Electricity and Magnetism I	C	50	50	100	3
MAT 10301	Multi Variable Calculus	C	50	50	100	4
MAT 10302	Mathematical Methods I	C	50	50	100	4
BIO 10302	Biology – III	C	50	50	100	3
ENV 10301	Environmental Science	C	50	50	100	2
CHE 10302	Chemistry Lab – Qualitative Analysis II	C	100	-	100	2
PHY 10302	Physics Lab – Electricity and Magnetism	C	100	-	100	2
BIO 10302	Biology Lab – III	C	100	-	100	2
	Total		600	300	900	25

SEMESTER – IV

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 10401	Introductory Physical Chemistry	C	50	50	100	3
PHY 10401	Quantum Physics and Relativity	C	50	50	100	3
MAT 10401	Mathematical Methods II	C	50	50	100	4
STA 10401	Statistics – Statistical Probability	C	50	50	100	4
BIO 10401	Biology – IV	C	50	50	100	3
COM 10401	Basic Computer Science	C	50	50	100	2
CHE 10402	Chemistry Lab – Physical Chemistry	C	100	-	100	2
PHY 10402	Physics Lab – Modern Physics	C	100	-	100	2
BIO 10402	Biology Lab – IV	C	100	-	100	2
	Total		600	300	900	25

SEMESTER – V

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 10501	Analytical Chemistry	C	50	50	100	2
CHE 10502	Inorganic Chemistry - Main Group Chemistry	C	50	50	100	3
CHE 10503	Chemical Kinetics and Thermodynamics	C	50	50	100	3
CHE 10504	Organic Functional Group Chemistry	C	50	50	100	3
CHE 10505	Elements of Symmetry and Molecular Spectroscopy	C	50	50	100	3
CHE 10506	Inorganic Chemistry Lab – Inorganic	C	100	-	100	2
CHE 10507	Organic Chemistry Lab – Synthesis and Separation	C	100	-	100	2
CHE 10508	Open Ended Lab - I	C	100	-	100	2
CHE 10509	Mathematics for Chemists	C	50	50	100	2
	Total		550	250	800	22

SEMESTER – VI

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 10601	Instrumental Methods of Analysis	C	50	50	100	2
CHE 10602	Coordination Chemistry and Organometallic Chemistry	C	50	50	100	3
CHE 10603	Electrochemistry, Solid State and Liquid State	C	50	50	100	3
CHE 10604	Organic Reactions and Mechanism	C	50	50	100	3
CHE 10605	Industrial Chemistry	C	50	50	100	3
CHE 10606	Chemistry Lab - Physical	C	100	-	100	2
CHE 10607	Chemistry Lab - Industrial	C	100	-	100	2
CHE 10608	Open Ended Lab - II	C	100	-	100	2
CHE 10609	Computer Programming and Numerical Methods	C	50	50	100	2
	Total		550	250	800	22

SEMESTER – VII

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 10701	Quantum Chemistry	C	50	50	100	3
CHE 10702	Structural Inorganic Chemistry of Main Group	C	50	50	100	3
CHE 10703	Statistical and Equilibrium Thermodynamics	C	50	50	100	3
CHE 10704	Stereochemistry	C	50	50	100	3
CHE 10705	Organic Photochemistry, Pericyclic Reactions and Rearrangements	C	50	50	100	3
CHE 107xx	Elective – I	E	50	50	100	2
CHE 10706	Physical Chemistry Lab	C	100	-	100	2
CHE 10707	Organic Chemistry Lab – Estimation and Separation	C	100	-	100	2
CHE 10708	Open Ended Lab - III	C	100	-	100	2
	Total		550	250	800	23

SEMESTER – VIII

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 10801	Group Theory and Spectroscopy	C	50	50	100	3
CHE 10802	Chemistry of Transition metals	C	50	50	100	3
CHE 10803	Chemical Kinetics and Surface Chemistry	C	50	50	100	3
CHE 10804	Reagents and Organic Synthesis	C	50	50	100	3
CHE 10805	Organic Spectroscopy	C	50	50	100	3
CHE 108xx	Elective – II	E	50	50	100	2
CHE 10806	Inorganic Chemistry Lab	C	100	-	100	2
CHE 10807	Organic Chemistry Lab - Multistep synthesis, purification and characterization	C	100	-	100	2
CHE 10808	Open Ended Lab - IV	C	100	-	100	2
	Total		550	250	800	23

SEMESTER – IX

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 10901	Organometallic and Bioinorganic Chemistry	C	50	50	100	3
CHE 10902	Advanced Solid State and Electrochemistry	C	50	50	100	3
CHE 10903	Chemistry of Natural Products	C	50	50	100	3
CHE 10904	Biological Chemistry	C	50	50	100	3
CHE 109xx	Elective – III	E	50	50	100	2
CHE 109xx	Elective – IV	E	50	50	100	2
CHE 10905	Computational Chemistry Lab	C	100	-	100	2
CHE 10906	Chemistry Lab - Instrumentational	C	100	-	100	2
CHE 10907	Open Ended Lab - V	C	100	-	100	2
	Total		600	300	900	22

SEMESTER –X

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 11001	Dissertation	C	-	100	100	18
CHE 11002	Viva	C	-	100	100	2
	Total		-	100	100	20

Elective Courses

Course Code	Name	C/E	Marks Distribution			Credit
			Continuous evaluation	End semester	Total	
CHE 10709	Chemistry of Polymers	E	50	50	100	2
CHE 10710	Materials Chemistry	E	50	50	100	2
CHE 10711	Advanced Equilibrium Thermodynamics	E	50	50	100	2
CHE 10712	Environmental Chemistry	E	50	50	100	2
CHE 10713	Biomolecules and Bioorganic Chemistry	E	50	50	100	2
CHE 10809	Quantum Chemistry of Molecules and Macromolecules	E	50	50	100	2
CHE 10810	Adsorption and Catalysis	E	50	50	100	2
CHE 10811	Crystallography	E	50	50	100	2
CHE 10812	Bioanalytical Chemistry	E	50	50	100	2
CHE 10908	Computational Chemistry	E	50	50	100	2
CHE 10909	Green Chemistry	E	50	50	100	2
CHE 10910	Electroanalytical Techniques	E	50	50	100	2
CHE 10911	Advanced Photochemistry	E	50	50	100	2
CHE 10912	Microbial Technology	E	50	50	100	2
CHE 10913	Advanced Solid-State Chemistry	E	50	50	100	2
CHE 10914	Polymer Technology	E	50	50	100	2
CHE 10915	Chemistry of Carbohydrates	E	50	50	100	2
CHE 10916	Medicinal Chemistry	E	50	50	100	2

CHE 10101: Atomic Structure and Chemical Bonding (3 credits, 48 hrs.)

UNIT -I (10 hrs.)

Dalton's Atomic Theory, Molecules, Chemical Nomenclature, Atomic and Molecular Mass, The Nucleus, Protons, Neutrons, and Electrons, Isotopes, Ions., Electromagnetic Spectrum, Line Spectra of Atoms, Photons, Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Double slit experiment, Heisenberg's uncertainty principle and its significance, Wave-Particle duality, de Broglie equation.

UNIT - II (10 hrs.)

Schrödinger's wave equation, significance of ψ and ψ^2, Quantum numbers and their significance. Sign of wave functions. Radial and angular wave functions. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Contour boundary and probability diagrams.

UNIT - III (8 hrs.)

Quantization, Electronic Transitions, Quantum Theory, Atomic Energy States, Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number. Electronic energy level diagram and electronic configurations of hydrogen-like and polyelectronic atoms and ions. Excited states.

UNIT - IV (10 hrs.)

Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Lande equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Solvation energy, Covalent bond, Lewis structure, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths, Ionic character in covalent compounds: Bond moment and dipole moment.

UNIT -V (10 hrs.)

Valence Bond theory, Hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. bonding, non-bonding, antibonding molecular orbitals (concept only) elementary pictorial approach of homo- and hetero-diatomic molecules H_2, B_2, C_2, O_2, N_2, CO, NO and CO_2, H_2O etc. molecular orbitals, sigma and pi bonds, multiple bonding, Concept of Bond order, bond length, bond strength, bond energy, Formal charge, Molecular Electron Configurations, Metallic Bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, Van der Waal's forces, ion-dipole, dipole–dipole interactions, London forces, Hydrogen bonding; Effect of chemical forces on physical properties.

Recommended Text Books:

1. Lee, J.D. Concise Inorganic Chemistry, 5th Ed., John Wiley & Sons, 1999.
2. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, 3rd Ed., Oxford, 1994.
3. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Ed., Oxford Press, 2006.
4. Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, 2nd Ed., ACS Publications, 2002.
5. Huheey, J. E., Keiter, E. A. and Keiter, R. L. Inorganic Chemistry, Principle and structure and reactivity, 4th Ed., Harper Collins College Publishers, New York, 1993.
6. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
7. Housecroft, C. and Sharpe, G., Inorganic Chemistry, 4th Ed., Pearson, 2012.
8. Levine, I. N. Physical Chemistry, 6th Ed., McGraw-Hill Education, 2008.

CHE 10102: Chemistry Lab – Quantitative Analysis I (Volumetric Analysis)

(2 credits, 64 hrs.)

Acidimetry and Alkalimetry

1. Strong acid- Strong base
2. Strong base -Weak acid
3. Strong acid-Weak base
4. Estimation of hardness of water

Permanganometry

1. Estimation of Oxalic acid
2. Estimation of Mohr's salt
3. Estimation of Ferrous iron
4. Estimation of Manganese dioxide in pyrolusite

References

1. Vogel's Textbook of Quantitative Chemical Analysis 6th Ed., Pearsons Education Ltd.
2. Laboratory Manual, CHE 10102, Department of Applied Chemistry, CUSAT

CHE 10201: Periodicity, Nuclear Chemistry, Acid Base Chemistry and Metallurgy

(3 credits, 48 hrs.)

UNIT – I **(10 hrs.)**

Atomic weights, Development of periodic law, The modern periodic table, Basis of periodic classification, orbital types and periodic table, Commonality in electronic configurations, Atomic sizes, ionization energy, Electron negativity, Electron Affinity, Polarizability and polarizing power, Relative orbital energies and overlap, Trends associated with properties – Physical and chemical, Anomalies in periodic properties. Predicting Chemistry of super heavy elements.

UNIT – II **(10 hr.)**

Nuclear radius, Nuclear Forces, Nuclear Spin, Magnetic dipole moment, Elementary Particles, Binding Energy, Nuclear models – Shell model- magic number, periodicity in nuclear properties, Liquid drop model – fission and fusion, Nuclear Stability, Exchange theory, n/p ratio, Nuclear Radiations, Nuclear reactions – , Types of nuclear reactions, Decay Kinetics, Half-life, Radioactive disintegration series. Fission: Fission products and Fission yield curve, Fission energy, theory of nuclear fission, nuclear reactor, breeder reactor - nuclear reactors in India. Fusion reactions, hydrogen bomb and energy of sun.

UNIT – III **(10 hrs.)**

Transuranium elements- Transuranium elements: Synthesis, separation and properties of transuranium elements. Radio isotopes: Co-precipitation, ion-exchange, solvent extract ion - as a tracer, Synthesis of labeled compounds (any two), isotopic dilution and radiopharmaceuticals. Neutron activation analysis, Principles of determination of age of rocks and minerals, radio carbon dating principles, Isotope dilution and neutron activation analysis.

UNIT – IV **(8 hrs.)**

Acid Base concepts, Bronsted-Lowry definition, Lux Flood Definition, Solvent system definition, Lewis Definition, Usanovich Definition, Generalized concept, Measures of acid base concept, Acid Base anomalies, HSAB theory.

UNIT – V **(10 hrs.)**

Occurrence of metals based on standard electrode potential, methods of concentration of ores, reduction to free metal, electrometallurgy, hydrometallurgy, and synthesis of ultrapure elements. Refining of metals, electrolytic, ion exchange, zone refining, vapour phase refining and oxidative refining. Thermodynamics of the oxidation of metals to metal oxides - Ellingham diagrams. Extractive metallurgy of U, Th, Ti.

Recommended Text Books:

1. D.M.P. Mingos, Essential trends in inorganic chemistry, Oxford University press 1998.
2. Gary Wulfsberg Inorganic Chemistry, VIVA, 2002.
3. N. N. Greenwood, A. Earnshaw, Chemistry of elements, Maxwell Macmillan Internatioanl editions, Pergamon Press, 1989.
4. Cotton, F.A., Wilkinson, G, Advanced Inorganic Chemistry. Wiley-VCH, 1999.
5. James E. Huheey, Ellen A. Keiter, Richard L. Kieter, Okhil K. Medhi, Inorganic Chemistry Principles Structure and Reactivity, Pearson Education, 4th edition, 2009.
6. B. K. Sharma, Industrial Chemistry (including Chemical Engineering), GOEL Publishing House, 1997.
7. H. J. Arnikar, "Essentials of Nuclear Chemistry", Wiley Eastern Ltd., New Delhi, 1982.

CHE 10202: Chemistry Lab – Qualitative Analysis I (Inorganic Mixture)

(2 credits, 64 hrs.)

Systematic qualitative analysis of mixtures containing two acid and two basic radicals from the list given below by semi micro method

Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, NH_4^+

CO_3^{2-}, SO_4^{2-}, NO_3^-, F^-, Cl^-, $C_2O_4^{2-}$, CH_3COO^-, PO_4^{3-}, CrO_4^{2-}

References

1. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
2. Laboratory Manual, CHE 10202, Department of Applied Chemistry, CUSAT

CHE 10301: Introductory Organic Chemistry (3 credits, 48 hrs.)

UNIT – I (7 hrs)

Nomenclature of organic compounds. Rules of IUPAC system of nomenclature of common organic compounds – alkanes, alkenes, alkynes, cycloalkanes, bicycloalkanes, alkyl halides, alcohols and phenols. Aldehydes, ketones, carboxylic acids and its derivatives, amines, nitro compounds.

UNIT – II (12 hrs)

Stereochemistry: Introduction, Concept of Isomerism, Classification of Stereoisomers, Optical isomerism, Chirality, Wedge formula, Fischer projection, Newman projection, perspective formula. Relative and absolute configurations, sequence rules, D & L, R & S systems of nomenclature. Enantiomers, meso form, diastereoisomers, epimers, anomers. Inversion, retention, racemization and resolution. Geometrical Isomerism: E-Z notation - determination of configuration. Conformational analysis: acyclic molecules, cyclohexane, substituted cyclohexanes- A values. Strain - types of strain including B, F, I, Pitzer strain, Beyer strain.

UNIT – III (9 hrs)

MOT and structures of organic molecules - I: Qualitative MOT. Group Orbitals of Methyl and Methylene groups. MO's of Methane, ethane, propane, methyl halides, ethylene, formaldehyde, conjugated systems: 1,3-butadiene, allyl radical, cation and anion. Structure and stability of reactive intermediates: classical and nonclassical carbocations, carbocations, carbanions, radicals, carbenes and nitrenes, benzyne, radical cations, radical anions, highly strained system (excluding reactions and synthetic applications).

UNIT – IV (8 hrs)

MOT and structures of organic molecules - II: Effects of pi conjugation: alkene, anion, cation and radical stabilizing groups, Hyperconjugation: effects of hyperconjugation with C-H bonds, C=C, lone pairs, cations, negative hyperconjugation, anomeric effect. Huckel's rule and modern theory of aromaticity. Study of [n]annulenes, super benzene, fullerenes, nonbenzenoid aromatics.

UNIT – V **(12 hrs)**

Basic introduction to Organic reactions - Electron displacement effects - Inductive, inductomeric, electromeric, mesomeric, hyper conjugation and steric effects - their influence on the physical and chemical properties of organic compounds. Nucleophilic substitutions - S_N1, S_N2, aromatic electrophilic substitution, Addition - polar and non-polar addition - addition of Bromine and hydrogen halides to double bonds - Markownikoff's rule and peroxide effect., Elimination - E1, E2, E1cb, pyrolytic elimination. Basic introduction to rearrangements and Pericyclic Reactions.

Recommended Text Books:

1. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Ed., Wiley, 2013
2. Carey, F. A. and Sundberg, R. J., Advanced Organic Chemistry (parts A and B), 5th Ed., Springer, 2008.
3. Bruice, P.Y. Organic Chemistry, 7th Ed., Prentice Hall Inc., 2013.
4. Morrison, R.T. Boyd, R.N. and Bhattacharjee, S.K. Organic Chemistry, 6th Ed., Pearson Education Inc., 2014.
5. Carroll, F.A. Perspectives on structure and mechanism in organic chemistry, 2nd Ed., Wiley, 2010.
6. Issacs, N. S. Physical Organic Chemistry, Second Edition, 2nd Ed., Prentice Hall, 1995.
7. Pross, A. Theoretical and Physical Principles of Organic Chemistry, 1st Ed., Wiley, 1995.
8. McMurry, J. Organic Chemistry, 5th Edition, Brooks/Cole, 2000.
9. Bruckner, R. Advanced organic chemistry: Reaction Mechanisms, 1st Ed., Academic Press, 2001.

CHE 10302: Chemistry Lab – Qualitative Analysis (Functional Group Analysis)

(2 credits, 64 hrs.)

Identification of simple organic compounds

Preparation of derivatives

Recommended Text Books:

1. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2nd Ed., 2007.
2. Dey, B.B. Sitaraman, M.V. and Govindachari, T.V. Laboratory Manual of Organic Chemistry, 3rd Ed., Viswanathan, 1957.
3. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Longman, 1989.
4. Mann, F.G. Saunders, B.C. Practical Organic Chemistry, 4th Ed., Pearson Education India, 2009.
5. Clark, H.T. A handbook of organic analysis, Longman, 1966.
6. Laboratory Manual, CHE 10302, Department of Applied Chemistry, CUSAT

CHE 10401: Introductory Physical Chemistry (3 credits, 48 hrs.)

UNIT – I (9 Hours)

Kinetic Theory of gases, Gas Laws, Ideal gas equation, Maxwell Distribution of velocity, Boltzmann distribution, Types of molecular velocities- r.m.s, most probable and mean velocity, Molecular Collisions, Mean free path,

Real gases- Deviation from ideal behavior- Compressibility factor, Van der Waals equation, Virial equation, PV isotherms, Continuity of states, Law of corresponding states, Critical phenomena and critical constants.

UNIT – II (10 Hours)

State functions, Reversible and irreversible processes, Isothermal and adiabatic processes, First, second and third laws of thermodynamics, Concepts of work, heat, Internal energy, enthalpy, Heat capacity, entropy, Gibbs energy, Helmholtz energy, Work done in isothermal and adiabatic reversible and irreversible processes, Joule Thomson effect- Inversion temperature, Application of J.T effect - Liquefaction of gases.

Entropy and free energy as criteria for spontaneity and equilibrium. Nernst Heat theorem and Unattainability of absolute zero.

UNIT – III (9 hours)

Rate laws, Order and molecularity, Zero, first, second and third order reactions- Integration of rate laws, Half life period, Arrhenius equation,

Photochemistry- Photochemical laws, Beer Lambert Law, Quantum yield, Jablonski Diagram -Photophysical and photochemical processes, Fluorescence, Phosphorescence-, Chemiluminescence, Bioluminescence, Photosensitisation, Photosynthesis

UNIT – IV (9 hours)

Theories of acids and bases- Arrhenius Theory, Lewis theory and Bronsted Theory, Hard and soft acids, pH, PK_a, PK_b, Ionic product of water, Common ion effect, Solubility product, Acid strength, Degree of hydrolysis of salts, Buffer solutions, Mechanism of buffer action, Henderson equation

UNIT - V (9 hours)

Surfaces and interfaces: Surface free energy and Surface tension, Contact angles and Wetting, Surface films. Adsorption- Physisorption and chemisorption, Adsorption Isotherms- Langmuir, Freundlich and BET isotherms (Qualitative approach), Application of isotherms

for surface area determination, Catalysis- homogeneous and heterogeneous (introduction) Colloids- Lyophilic and Lyophobic colloids, Preparation of colloids, Kinetic, optical and electrical properties, Electrical double layer Models for double layer: Heimboltz, Gouy- Champman and Stern, Zeta potential. Stability of colloids, Protective colloids- Gold number, Flocculation, Hardy Schulze rule, Surfactants, micelles, Donnan membrane equilibrium, Dorn effect, Sedimentation potential and streaming potential, Emulsions, Gels, Sols.

Recommended Text Books:

1. Ira.N.Levine, Physical Chemistry, Tata Mc Graw Hill, 6th Ed., 2009
2. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, 10th Ed., 2017.
3. K J Laidler, J.H Meiser, Physical Chemistry, 4th Ed., 2003.
4. Donald McQuarrie & John Simon, Physical Chemistry, A molecular approach, Oxford University Press, 2006
5. R.A.Alberty & R.J.Silbey, Physical Chemistry, Wiley Publishers, 4th Ed., 2004

CHE 10402: Chemistry Lab - Physical Chemistry (2 credits, 64 hrs.)

pH METRY

Strong acid X strong base, Strong acid X weak base, Weak acid X Strong base

POTENTIOMETRY

Strong acid X strong base, Strong acid X weak base, Weak acid X Strong base, $KMnO_4$ X Fe^{2+}

CONDUCTOMETRY

Strong acid X strong base, Strong acid X weak base, Weak acid X Strong base

COLORIMTERY

Estimation of iron, chromium, nickel, Manganese, Copper, phosphate in soft drinks

Recommended Text Books:

1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan, 2014.
2. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. Laboratory Manual, CHE 10402, Department of Applied Chemistry, CUSAT

CHE 10501: Analytical Chemistry **(2 credits, 32 hrs.)**

UNIT – I **(8hours)**

Significant figures, Accuracy, Precision, Error, Types of errors- Determinate and Indeterminate errors, Distribution of random errors, Mathematical Expression for error- Absolute and Relative error, Methods to reduce error, Statistical tools for expressing precision- Standard deviation, Relative standard deviation, Variance, Comparison of results- Students t test, f test, Criteria for rejecting a value-Q test, Confidence interval, Correlation and Regression, Linear regression analysis

UNIT – II **(6 hours)**

Titrimetric analysis and calculations, Different types of titrations - neutralization, redox (permanganometry, dichrometry, iodometry, iodimetry), complexometric (EDTA titrations) and precipitation titrations – Principle of all types of titrations, titration curves, indicators.

Gravimetric analysis – Illustration using barium and iron estimation.

UNIT – III **(6 hours)**

Potentiometry – Principle, Indicator electrode, different types of indicator electrodes, Reference electrodes, Potentiometric titrations

UNIT – IV **(6 hours)**

Voltammetry, Excitation signals in voltammetry, Instrumentation, Polarography, Ilkovic equation, half wave potential Cyclic voltammetry, Pulse voltammetry, Amperometry, Applications of voltammetry

Electrogravimetric methods and coulometric methods

UNIT – V **(6 hours)**

Solvent extraction, Solid phase extraction, Electrophoresis

Chromatography- Selection of mobile and stationary phase, TLC, Column chromatography Gas chromatography, HPLC, Supercritical fluid chromatography, Ion exchange chromatography, Size exclusion chromatography

Recommended Text Books:

1. Skoog, West, Holler, Crouch, Fundamentals of Analytical Chemistry, 9th Edn.
2. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, 5th Edn.
3. James W. Robinson, Eileen M. Skelly Frame, George M. Frame II, Undergraduate Instrumental Analysis
4. Vogel's textbook of quantitative chemical analysis, 6th edn

CHE 10502: Inorganic Chemistry - Main Group Chemistry (3 credits, 48 hrs.)

UNIT – I (10 hrs.)

s- Block elements- Hydrogen, Hydrogen Bonding, Hydrates, Hydrogen ions, acids and bases, Properties of - Hydro Halic acids, Nitrous acid, perchloric acids, sulphuric acids, and metal hydrides. Group 1 elements-- General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Flame colors and spectra, Color of compounds, Alkali metals in liquid ammonia and other solvents, Oxides, Hydroxides, hydrides, alkoxides, amido complexes, Ionic salts and M^+ ions in solution, Alkali metal complexes. Group 2 elements – - General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Elemental Beryllium, Binary Compounds, Coordination compounds with oxygen and nitrogen ligand, organoberyllium compounds, Compounds of Magnesium, calcium, strontium-, oxides, halides, hydrides, carbides, ionic salts and complexes, alkoxides.

UNIT – II (12hrs.)

p- Block elements – Group 13 elements- General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, oxides, halides, Complex Compounds, Chemistry of oxidation states I and II, Boranes- Preparation, Classifications, Structure and Bonding, Tetrahydroborate ion, Boron Halides, Boron – Nitrogen Compounds, Boron – Oxygen Compounds. Group 14 elements – General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Carbon- Properties, Allotropes, Carbon Halides, Carbon Oxides, Compounds with C-N bond, C-S bond, Carbon compounds as ligands. Oxygen compounds of Silicon, Organo compounds, Silanes and Silenes, Inorganic Polymers, Nanotechnology.

UNIT – III (9 hrs.)

Group 15 elements - General Behavior, Occurrence and abundance, Group trends and stereochemistry, Electronic Configuration and types of bonding, Active Nitrogen, Nitrogen fixation natural and artificial, Nitrogen compounds- Nitrides, Ammonia, Hydrazine, Oxides of Nitrogen, Oxo acids and anions, Halogen Compounds, nitrogen compounds as ligands,

Halides of Phosphorous, Oxides of Phosphorous, Sulfides and other chalcogenides of phosphorous, Phosphonium, Phosphorous – Nitrogen Compounds, Organic compounds of Phosphorous, Compounds with element-element bonds, Oxo anions of Phosphorous, Phosphate in bio systems, Phosphorous compounds as ligands, Compounds of Ar, Sb and Bi.

UNIT – IV **(9 hrs.)**

Group 16 elements - General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Group trends and stereochemistry, Types of oxides, Chemical properties of Dioxygen, Singlet oxygen, ozone, Peroxo compounds, Superoxide, Halo compounds, Oxygen compounds as ligands, Sulfanes, polysulfides, Sulphur- Nitrogen Compounds, Halogen compounds of sulphur, Oxides, oxohalides and oxo acids of Sulphur , Sulphur compounds as ligands.

UNIT – V **(8hrs.)**

Group 17 elements- General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Preparation, C-T complexes of Halogen, Halides, Molecular halides, Halides and halogen compounds as ligands, Oxides and oxo acids, Interhalogen and poly halogen compounds, Oxohalogen fluorides. Group 18 elements - General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Halogen compounds.

Recommended Text Books:

1. D.M.P. Mingos, Essential trends in inorganic chemistry, Oxford University press 1998.
2. Gary Wulfsberg Inorganic Chemistry, VIVA, 2002.
3. N. N. Greenwood, A. Earnshaw, Chemistry of elements, Maxwell Macmillan Internatioanl editions, Pergamon Press, 1989.
4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. Wiley-VCH, 1999
5. James E. Huheey, Ellen A. Keiter, Richard L. Kieter, Okhil K. Medhi, Inorganic Chemistry Principles Structure and Reactivity, Pearson Education, 4th edition, 2009.
6. J.D. Lee, A Concise Inorganic Chemistry, ELBS.

CHE 10503: Chemical Kinetics and Thermodynamics (3 credits, 48 hrs.)

UNIT – I (9 hours)

Overall review of rate equations, order and molecularity, Half life and temperature dependence of rate constant. Complex Reactions- Parallel, Consecutive and Opposing reactions, Steady state Approximation, Theories of Reaction Rate- Collision Theory and Activated Complex Theory- Collision and reaction cross section, PES, Erying Equation, Theory of unimolecular reactions- Lindemann Mechanism, Kinetics of chain reactions - Photochemical reactions H_2-Cl_2 and H_2-Br_2 reaction, Organic decomposition reactions-Rice Herzfield mechanism (acetaldehyde and ethane), Branched Chain Reactions, Explosions-Somenoff Hinshelwood mechanism (H_2-O_2 reaction), Termolecular reactions.

Study of Fast Reactions- Relaxation Methods, Flash photolysis

UNIT – II (9 hours)

Review of laws of thermodynamics, Residual entropy, Criteria of spontaneity in terms of entropy and free energy, Entropy and free energy changes during isothermal and adiabatic processes, Changes in entropy and free energy with Temperature and pressure, Gibbs Helmhotlz equation, Maxwells Relations, Partial molar properties, Chemical potential, Gibbs Duhem equation and Duhem Margules equation, Thermodynamics of mixing, Concept of fugacity and activity- determination.

UNIT – III (9 hours)

Equilibrium constants in terms of concentration, partial pressure and mole fraction, Le Chateliers principle and application to physical and chemical equilibria, Enthalpy changes in chemical reactions, Born Haber cycle, Hess's Law, Kirchoff equation, Applications of free energy to physical and chemical changes. Effect of temperature and pressure on chemical equilibrium- vant Hoff reaction isotherm and isochore.

UNIT – IV (10 hours)

Gibbs phase rule, Application to one component, two component systems – Water, Helium and Sulphur systems, Simple eutectic system, Deep eutectic solvents, Compound formation with congruent and incongruent melting point, Salt hydrate-water systems, Freezing mixtures, Three component systems involving three liquids and two solids and a liquid

UNIT – V **(9 Hours)**

Concept of Molarity, molality, Normality. Raoults law, Henrys law, Deviation from ideality – Ideal, real and regular solutions, Excess functions, Binary systems of completely miscible liquids-Vapour pressure-composition diagram, Boiling point-composition diagram, Fractional distillation of binary solutions, Colligative properties- elevation in b.p, depression in f.p, osmotic pressure, Abnormal molecular mass- vant Hoff factor

Liquid- vapour equilibrium and solid- vapour equilibrium- Clausius Clapeyron equation, Liquid-liquid equilibrium- partially miscible liquid systems- CST, Immiscible liquid systems- Nernst distribution law- Derivation and Applications, Principle of Steam distillation.

Recommended Text Books:

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, 3rd edn, 1981.
2. K. J. Laidler, Chemical-Kinetics, Low price edn., 2003.
3. F. Daniels and R. A. Alberty, Physical Chemistry, Wiley Publishers, 4th edn 2004
4. Peter Atkins and Julio de Paula, Physical Chemistry, Oxford University Press, 10th edn, 2017.
5. I.M.Klotz & R.M.Robsenberg "Chemical Thermodynamics", Wiley, 7th Edn, 2008.
6. L.K.Nash, "Elements of Chemical Thermodynamics" Addison Wesley, 2nd edn, 2013.

CHE 10504: Organic Functional Group Chemistry (3 credits, 48 hrs.)

UNIT – I (6 hrs.)

Akyl and aryl halides - Classification, physical properties, preparation methods, reactions.

UNIT – II (10 hrs.)

Alcohols, phenol and ethers - Classification, physical properties, preparation methods, reactions – with hydrogen halide, order of reactivity of 1^o, 2^o and 3^o alcohols, with PCl_3, dehydration, with active metals, ester formation, formation of alkyl sulfonates, oxidation – primary, secondary and tertiary alcohols, chemoselective oxidants for alcohols – Oppenauer's oxidation, Moffatt-Pfitzner oxidation, Des-Martin oxidation, Alcohols as acids and bases. Ascent and decent in alcohol series Dihydric alcohols: Oxidative cleavage – Lead tetra acetate, Periodic acid- Pinacol - Pinacolone rearrangement –mechanism.

Phenols - Preparation, physical properties, - Acidity of phenols, reactions, rearrangement of phenol derivatives-Fries rearrangement, Claisen rearrangement

Ethers – preparation, physical properties, reactions – cleavage by acids. Synthesis and Reactions of Epoxides, Cleavage of ether linkages by HI- Ziesels method of estimation of methoxy groups.

UNIT – III (14 hrs)

Aldehydes, Ketones, acids and their derivatives

Physical properties, preparation, reactions – Cannizaro reaction, Aldol condensation, Wittig reaction, nucleophilic addition - addition of cyanide, derivatives of ammonia, Grignard reagent, alcohols, oxidation and reduction – Baeyer-Villiger oxidation-Cannizzaro's reaction, Meerwein-Ponndorf Verley reduction, Clemmensen reduction, Wolff-Kishner reduction, $LiAlH_4$ and $NaBH_4$ reductions., α, β – unsaturated carbonyl compounds – Claisen, Claisen-Schmidt, Dieckmann, Benzoin, Aldol, Perkin and Knoevenagel condensations, nucleophilic and electrophilic addition – Michael addition and Robinson annulation, Mannich reaction

Carboxylic Acids and acid chlorides & esters

Physical properties – Acidity of carboxylic acids – effect of substituents, preparation, reactions – salt formation and decarboxylation, preparation and reactions of functional derivatives, halogenation of aliphatic acids - Hell-Volhard- Zelinsky reaction.

Methods of formation and chemical reactions of anthranilic acid, cinnamic acid, acrylic acid, oxalic acid, malonic acid, citric acid, adipic acid, maleic acid, fumaric acid. Preparation and reactions of benzene sulphonic acid, benzene sulphonyl chloride and otho and para toluene sulphonyl chlorides- uses. Esters, hydroxyl acids, lactones.

Compounds containing active methylene groups

Synthetic uses of malonic ester, acetoacetic ester and cyanoacetic ester. Keto-enol tautomerism of ethyl acetoacetate Alkylation of carbonyl compounds via enamines.

UNIT – IV **(10 hrs)**

Nitrogen containing compounds

Amines- isomerism- stereochemistry of amines, distinguish between primary, secondary and tertiary amines- Structural features affecting basicity of aliphatic and aromatic amines. Quaternary amine salts as phase-transfer catalysts. Comparative study of aliphatic and aromatic amines. Preparation of alkyl and arylamines (reduction of nitro compounds, nitriles), reductive amination of aldehydic and ketonic compounds, Gabriel-Phthalimide reaction, Diazonium salts-preparation, synthetic transformations of aryl diazonium salts, azo coupling-. Mechanisms of Sandmeyer's and Gatterman reactions- Schiemann and Gomberg reactions Preparation and uses of Phenyl hydrazine. Diazomethane and diazoacetic ester - preparation, structure and synthetic uses.-Arndt Eistert synthesis- mechanism –Wolff rearrangement.

Amides - preparation and reactions.

Unit – V **(8 hrs.)**

General introduction to carbohydrates: monosaccharides, disaccharides, mutarotation, glyoxal, stepping up and stepping down, reducing and non-reducing sugar, glycosidic linkage, O & N glycosides.

Aminoacids and lactams (α, β, γ etc.) urea, thiourea, guanidine.

Recommended Text Books:

1. Bruice, P.Y. Organic Chemistry, 7th Ed., Prentice Hall Inc., 2013.
2. Morrison, R.T. Boyd, R.N. and Bhattacharjee, S.K. Organic Chemistry, 6th Ed., Pearson Education Inc., 2014.
3. Clayden, J. Green, N. Warren, S. and Wothers, P. Organic Chemistry, 2nd Ed., Oxford University Press, 2012
4. McMurry, J. Organic Chemistry, 5th Ed., Brooks/Cole, 2000.
5. Bruckner, R. Advanced Organic Chemistry: Reaction Mechanisms, 1st Ed., Academic Press, 2001.
6. Carey, F.A. and Sundberg, R.J. Advanced Organic Chemistry (parts A and B), 5th Ed., Springer, 2008.
7. Norman, R.O.C. Principles of Organic Synthesis, 2nd Ed., Chapman and Hall, 1978.
8. Solomons, T.W.G. Fryhle, C.B., Snyder, S. A. Organic Chemistry, 12th Ed., Global, 2017.

CHE 10505: Elements of Symmetry and Molecular Spectroscopy

(3 credits, 48 hrs.)

UNIT – I **(10 hrs.)**

Symmetry as a universal theme. Different symmetry classes and symmetry operations (discussion with suitable examples). Applications of symmetry to a) Polar molecules b) chiral molecules. Symmetry properties of orbitals (basic concepts); concept of point groups, identification of molecular point groups in some simple molecules.

UNIT – II **(8 hrs.)**

Spectroscopy and its importance in chemistry. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. origin of linewidths in molecular spectra, Transition dipole moment and Fermi's Golden Rule, Einsteins Coefficients, Lasers and Masers; Types of spectroscopy. Difference between atomic and molecular spectra. Separation of molecular energies into translational, rotational, vibrational and electronic components. Born-Oppenheimer approximation, Postulates of quantum mechanics, quantum mechanical operators.

UNIT – III **(10 hrs.)**

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels. Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy. determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

UNIT – IV **(10 hrs.)**

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). concept of zero-point energy. Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies.

Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.

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.

UNIT – V **(10 hrs.)**

Electronic Spectroscopy: Electronic excited states. Free Electron model, its application to electronic spectra of polyenes. Franck-Condon principle, electronic transitions, Beer Lambert's Law, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

Recommended Text Books:

1. Banwell, C. N. and McCash, E. M. Fundamentals of Molecular Spectroscopy, 4th Ed. Tata McGraw-Hill: New Delhi, 2006.
2. Kemp, W. Organic Spectroscopy, 3rd Ed., Palgrave, 1991.
3. Barrow, G. M. Physical Chemistry, 6th Ed., McGraw-Hill College, 1996.
4. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Ed., Oxford Press, 2006.
5. Levine, I. N. Physical Chemistry, 6th Ed., McGraw-Hill Education, 2008.
6. Cotton, F. A. Chemical Applications of Group Theory, 3rd Ed., Wiley Interscience, New York, 2008.
7. Gopinathan, M. S. and Ramkrishnan, V. Group Theory in Chemistry, 2nd Ed., Vishal Publishing Co., 2013.

CHE 10506: Inorganic Chemistry Lab (Volumetry and Gravimetry)

(2 credits, 64 hrs.)

Complexometry

1. Estimation of Zinc
2. Estimation of Magnesium
3. Estimation of different metal ions from a mixture – use of masking agents

Gravimetric analysis

1. Estimation of Barium/sulphate as Barium sulphate
2. Estimation of iron as Ferric oxide
3. Estimation of Nickel

Recommended Text Books:

1. Vogel's Textbook of Quantitative Chemical Analysis 6th Ed., Pearsons Education Ltd.
2. Laboratory Manual, CHE 10506, Department of Applied Chemistry, CUSAT

CHE 10507: Organic Chemistry Lab (Synthesis and Separation) (2 credits, 64 hrs.)

One step synthesis of Organic Compounds

Separation of organic mixtures by TLC, GC

Recommended Text Book:

1. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2nd Ed., 2007.
2. Dey, B.B. Sitaraman, M.V. and Govindachari, T.V. Laboratory Manual of Organic Chemistry, 3rd Ed., Viswanathan, 1957.
3. Furniss, B.S. Hannaford, A.J. Smth, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Longman, 1989.
4. Mann, F.G. Saunders, B.C. Practical Organic Chemistry, 4th Ed., Pearson Education India, 2009.
5. Clark, H.T. A handbook of organic analysis, Longman, 1966.
6. Laboratory Manual, CHE 10507, Department of Applied Chemistry, CUSAT.

CHE 10508: Open Ended Lab **(2 credits, 64 hrs.)**

CHE 10509: Mathematics for Chemists **(2 credits, 32 hrs.)**

UNIT – I **(5 hrs.)**

Numbers: Real and Complex number algebra. Vector algebra.

UNIT – 2 **(7 hrs.)**

Functions & Variables: Differential calculus-first- and higher-order derivatives, evaluation of minimum and maximum, limits & continuity. Partial differentiations. Exact and inexact differentials. Numerical differentiation. The gamma and delta functions.

Integral Calculus: Indefinite and definite integrals, improper integrals. Methods of integration. Surface and volume integrals. Numerical integrations.

UNIT – 3 **(7 hrs.)**

Differential Equations: Ordinary first- and second-order differential equations. Partial differential equations. Solution of inexact differential equations by the method of integrating factors. Power series and extended power series solutions. Numerical solutions.

UNIT – 4 **(6 hrs.)**

Special functions: Hermite, Legendre and Laguerre polynomials, recursion relations.

Matrices and Determinants. Eigenvalues and eigenvectors. Orthogonal transformation. Rank & inverse of matrix.

UNIT – 5 **(7 hrs.)**

Solution of Linear Systems: Gaussian elimination, Cramer's rule. Gauss-Jordan elimination. Gauss-Seidel and Jacobi methods. Solution of non-Linear Systems: Newton-Raphson method.

Curve fittings. Permutation & Combination. Probability. Stirling's approximation. Lagrange multipliers.

Text Books

1. R. G. Mortimer, Mathematics for Physical Chemistry. 3rd Edn., Academic Press. 2014

2. E. Kreyszig, Advanced Engineering Mathematics. 9th Edn. Wiley, 2015

3. G. Turrell, Mathematics for Chemistry and Physics, 2nd Edn., Academic Press, 2004

4. D. A. McQuarrie, Mathematics for Chemists and Physicists, 4th Edn., Wiley, 2007

CHE 10601: Instrumental Methods of Analysis **(2 credits, 32 hrs.)**

UNIT I **(6 hours)**

Optical systems used in spectroscopy – Sources, Filters, Monochromators, Detectors, Single and Double beam optics, Signal to noise ratio, bandwidth and band pass

UNIT II **(6 hours)**

Atomic absorption spectroscopy – Absorption of radiant energy by atoms, Instrumentation, Interferences in AAS, Analytical applications of AAS

Atomic Emission spectroscopy – Principle – Types – Flame atomic emission spectroscopy, Flame photometry, Plasma emission spectroscopy

UNIT III **(6 hours)**

Rotational spectroscopy – Instrumentation

Vibrational spectroscopy – Instrumentation, advantages of FT IR

Laser Raman spectroscopy – Instrumentation

UV –Visible, NIR and Far IR - Instrumentation

Molecular fluorescence spectroscopy- Theory, instrumentation and applications

UNIT IV **(8 hours)**

NMR – Principle, common spin ½ nuclei, chemical shift, shielding and deshielding, anisotropic effects, Basic instrumentation

ESR - Principle, Hyperfine interactions, Basic instrumentation

Principle and instrumentation of UPS, XPS, Mossbauer spectroscopy

UNIT V **(6 hours)**

Overview of SEM, AFM and TEM, XRD and their applications

Gas and Liquid chromatography –Instrumentation, different types of detectors

Hyphenated techniques – GC-MS and LC-MS.

Recommended Text Books:

1. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, 5th Edn, Blackwell Science, 2000.
2. James W. Robinson, Eileen M. Skelly Frame, George M. Frame II, Undergraduate Instrumental Analysis, 7th Edn., CRC Press, Tailor and Francis group, 2014.
3. P. F. Bernath, Spectra of Atoms and Molecules, III Edn, Oxford University Press
4. I. N. Levine, Molecular Spectroscopy, John Wiley & Sons
5. Harald Gunther, NMR spectroscopy: Basic principles, Concepts and Applications in chemistry, 3rd edn, 2013.
6. J..Michael Hollas, Modern Spectroscopy, John Wiley & Sons
7. W. W. Parson, Modern Optical Spectroscopy, Springer-Verlag, 2007
8. C. Giacavazzo (Ed.) Fundamentals of crystallography, II edn., Oxford University Press, 2002.
9. J. D. Dunitz, X-ray analysis and the structure of organic molecules, II Edition, Wiley VCH, 1996.
10. G.H. Stout, L.H. Jensen, X-ray structure determination: A practical guide, II Edn., John Wiley and Sons, New York, 1989.
11. A. Braithwait, F. J. Smith, Chromatographic methods, 5th Edn., Kluwer Academic Publihers, 1999.

CHE 10602: Coordination Chemistry and Organometallic Chemistry

(3 credits, 48 hrs.)

UNIT – I **(8 hrs.)**

General periodic trends, Metallic property, Chemistry of variable oxidation states, properties of d configuration - d^0 to d^{10}, Type of compounds, absorption spectra, magnetic property. Lanthanides and Actinides- Stable oxidation states, lanthanide and actinide contraction, Occurrence and recovery; Separationof Lanthanides; difference between 4f and 5f orbitals, Type of compounds, absorption spectra, magnetic property.

UNIT – II **(10 hrs.)**

Werner's theory, Bonding in coordination compounds: Valence bond description and its limitations. valence bond theory (inner and outer orbital complexes), Crystal Field Theory (CFT). measurement of 10 Dq (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δ_o, Δ_t). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, Jahn – Teller effect in octahedral complexes, square planar geometry. Factors affecting the crystal-field parameters. Spectrochemical series, colour and spectral behaviours. magnetism of first – row transition metal complexes, stabilization of unusually low and high oxidation states of metals, Qualitative aspect of Ligand field and MO Theory, back bonding. Structural and stereoisomerism in complexes with coordination numbers 4 and 6.

UNIT – III **(10 hrs.)**

Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p, and multicentre bonds), metal-metal multiple bonding, Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, EAN rule as applied to carbonyls, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. Preperation and Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni. π-acceptor behaviour of CO, 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. Organo-lithium aluminium, magnesium, zinc and titanium compounds – their preparations, properties, reactions, bonding and applications. "Sandwitch'' compound: Ferrocene – its preparation, reactions and structure.

UNIT – IV **(10 hrs.)**

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, chelating ligands and macro-cyclic ligands, EDTA, porphyrin, crown-ether.

UNIT – V **(10 hrs.)**

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium/K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine. Iron and its application in bio-systems, Haemoglobin; Storage and transfer of iron. heme and non-heme oxygen carriers, haemoglobin and myoglobin-cooperativity; Bohr effect, Hill coefficient, oxy and deoxy haemoglobin, reversible binding of oxygen.

Recommended Text Books:

1. Purcell, K.F & Kotz, J.C. Inorganic Chemistry, 2nd Ed., W.B. Saunders Co, 1991.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L. Inorganic Chemistry, Principle and structure and reactivity, 4th Ed., Harper Collins College Publishers, New York, 1993.
3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry 2nd Ed., University Science Books, 1994.
4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. 6th Ed., Wiley-Interscience, 1999.
5. Basolo, F, and Pearson, R.C., Mechanisms of Inorganic Chemistry, 2nd Ed., John Wiley & Sons, NY, 1967.
6. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, 2nd., Ed. Butterworth-Heinemann,1997.
7. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
8. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint, Pearson Education, 2005.
9. Douglas, B. E.; McDaniel, D.H. and Alexander, J.J. Concepts and Models in Inorganic Chemistry 3rd Ed., John Wiley and Sons, NY, 1994.

10. Powell, P. Principles of Organometallic Chemistry, 2nd Ed., Springer, 1991.
11. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
12. Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals. 6th Ed., New York, NY: John Wiley, 2014.
13. W. L. Jolly, Modern Inorganic Chemistry, McGraw-Hill International, 2nd Edition, New York, 1991.

CHE 10603: Electrochemistry, Solid State and Liquid State

(3 credits, 48 hrs.)

UNIT – I **(9 hours)**

Specific, equivalent and molar conductance, Faradays Law, Transport number and its determination, Kohlrausch's law, Ostwalds dilution law. Debye Huckel Onsager equation for strong electrolytes (No derivation), Applications of conductance measurement, Electrodes and Electrode potentials, Types of electrodes- Standard hydrogen electrode, Calomel electrode, Quinhydrone electrode, Standard electrode potential, Electrochemical series, Ionic mobility, Transport number and its determination- Hittorf's method and moving boundary method.

UNIT – II **(12 hours)**

Galvanic cells, Cell representation, Thermodynamics of reversible cells and electrodes- Determination of ΔH, ΔS and ΔG of cell reactions, EMF and equilibrium constant of cell reaction, Nernst Equation.

Liquid Junction Potential, Concentration cells - Electrode concentration cells and electrolyte concentration cells, Concentration cells with and without transference, Liquid junction potential, Applications of emf measurement- Determination of solubility product and activity co-efficient, pH determination, Potentiometric titrations, Redox indicators- principle. Overvoltage (Elementary idea)

Corrosion of metals- different forms of corrosion and prevention. Electrochemical Theory of corrosion.

Fuel cells- Hydrogen oxygen fuel cell, methanol fuel cells

UNIT – III **(9 hours)**

Crystal structures and symmetry, Crystallographic point groups, space group, unit cells, Miller indices, Seven crystal systems and Bravais lattices, Simple, body centered and face centered systems, Packing in solids- packing diagrams, close packing,- hcp and ccp structures, XRD, Braggs equation – derivation, Powder and rotating crystal technique. Identification of cubic crystals based on interplanar ratio.

UNIT – IV **(12 hours)**

Ionic solids with formula MX (CsCl, NaCl, Zinc Blende and Wurtzite Structures), MX_2 (Fluorite and Antfluorite Structures, Cadmium Halides, CaF_2, Rutile, Anti-rutile, beta-cristobalite), other crystal systems (Bismuth tri-iodide, Corundum, Rhenium Trioxide etc.), Mixed oxides (Spinel, Perovskite, Ilmenite).

Electronic Structure of Solids: Free electron theory and band theory, Concept of Fermi level, Hall effect, Semiconductors, extrinsic and intrinsic semi conductors, Superconductivity (Elementary information)

Point Defects in crystals- stoichiometric and non stoichiometric defects

Liquid Crystals- Classification and application.

UNIT – V **(6 hours)**

Vapour pressure , Surface tension - determination of vapour pressure. Parachor – determination, application to structure elucidation of compounds, Viscosity -determination of molecular mass from viscosity measurements. Refraction – refractive index, molar refraction and optical exaltation – application to structure elucidation, Concept of superhydrophobicity/superoleophilcity.

Recommended Text Books:

1. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Edn., Wiley, New York, 1998
2. 2. R. Crow, Principles and Applications of Electrochemistry, Paper back edn, 4th edn, 1994.
3. S.Glasstone, An Introduction to Electrochemistry, Paperback edn., 2007
4. L.V.Azaroff, Introduction to Solids, Mc Graw Hill, 1960.
5. A. R. West, Solid State Chemistry, Wiley Student (Indian) Ed., (2014)
6. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967.
7. Lesley Smart and Elaine Moore, Solid State Chemistry, Chapman and Hall, 1995.
8. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.
9. C. N. R. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry. 2nd edn, Cambridge Uty Press, 1997.

CHE 10604: Organic Reactions and Mechanism (3 credits, 48 hrs.)

UNIT – I (10 hrs)

Structure activity relationship and Determination of reaction mechanism: Guidelines on Pushing of electrons. Methods of determining reaction mechanisms (kinetic and non kinetic methods): The Hammond postulate, reactivity vs. selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs. thermodynamic control. Isotope effects.

Carbon acids: pKa of weak acids, Effect of structure on acidity and basicity. Linear free energy relationships: Hammett and Taft parameters, Solvent effects, nucleophilicity and nucleofugality. Other Experimental techniques to determine reaction mechanisms: identification of intermediates by trapping and competition experiments, cross - over experiments, isotope scrambling, radical clocks and traps, matrix isolation.

UNIT – II (9 hrs)

Application of Frontier Orbital theory: HSAB concept, Perturbation theory of reactivity. Application of Frontier Orbital theory in studying ionic reactions: aliphatic nucleophilic substitution reactions, Ambident nucleophiles, Ambident electrophiles, α-effect. Application of Frontier Orbital theory in studying radical reactions.

UNIT – III (11 hrs)

Substitution on aliphatic carbon: Mechanisms of Nucleophilic, Electrophilic and free radical substitution reactions on aliphatic carbons (saturated and unsaturated): Role of substrate structure, nature of reagents, nature of solvents and stereochemistry on the outcome of these reactions. Neighbouring group participation. Nonclassical carbocation.

UNIT – IV (9 hrs)

Substitutions on aromatic carbon: Mechanism of electrophilic, nucleophilic and free radical substitutions. Synthetic applications.

UNIT - V (9 hrs)

Addition and Elimination: Mechanisms of polar and nonpolar additions and eliminations (except pericyclic reactions). Addition and elimination via free radical intermediates, E2, E1

and E1CB mechanisms, Orientation and stereochemistry in E2 eliminations. Pyrolytic syn eliminations, α- eliminations, elimination vs. substitution.

Recommended Text Books:

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Ed., Wiley, 2013.
2. Lowry, T H. and Richardson, K.S. Mechanism and Theory in Organic Chemistry, 3rd Ed., Benjamin-Cummings Publishing Company, 1997.
3. Carey, F. A. and Sundberg, R. J., Advanced Organic Chemistry (parts A and B), 5th Ed., Springer, 2008.
4. Anslyn, E.V. and Dougherty, D.A. Modern Physical Organic Chemistry. University Science Books, 2005.
5. Carroll, F.A. Perspectives on structure and mechanism in organic chemistry, 2nd Ed., Wiley, 2010.
6. Issacs, N. S. Physical Organic Chemistry, Second Edition, 2nd Ed., Prentice Hall, 1995.
7. Pross, A. Theoretical and Physical Principles of Organic Chemistry, 1st Ed., Wiley, 1995.
8. Clayden, J. Green, N. Warren, S. and Wothers, P. Organic Chemistry, 2nd Ed., Oxford University Press, 2012.
9. Flemming, I. Frontier orbitals and organic chemical reactions, Wiley-Blackwell, 1976.
10. Flemming, I. Molecular orbitals and organic chemical reactions, student edition, Wiley 2009.
11. McMurry, J. Organic Chemistry, 5th Edition, Brooks/Cole, 2000.
12. Bruckner, R. Advanced organic chemistry: Reaction Mechanisms, 1st Ed., Academic Press, 2001.

CHE 10605: Industrial Chemistry **(3 credits, 48 hrs.)**

UNIT – I **(10 hrs.)**

Source of Chemicals, Organic Chemicals, Inorganic Chemicals, Recycling of materials, waste minimization, E factor and atom economy, Reduction of- material use. Water management – water for industry, sources of water, water conditioning methods, municipal waste water, Industrial waste water – treatment. Energy Management- energy required by chemical industries, sources of energy, cost of energy, types of energy requirement, use of energy, efficient utilization of energy., energy, risk and hazards. Sustainable use of- chemical feedstocks, water, energy. Environmental pollution control – methods of pollution control, economics of pollution control, industrial health and hygiene.

UNIT – II **(8hrs.)**

Industrial Processes in practice – Basic chemical data, Flow charts; chemical process selection, design and operation, Plant location, safety, construction of plant, process system engineering. Case study of chemical industry of regional importance. Pharmaceutical Industries – Classification, methods of preparation, radioisotopes in medicine, biological hormones, steroids, vitamins, plant and animal isolates, drug design (basic understanding)

UNIT – III **(10hrs.)**

Fuel Industries – Calorific value, modern concept of fuels, classification, criteria for selection, comparison of gas, liquid and solid fuels, properties, methods of processing various fuels, solid fuels , Gaseous fuels, Petroleum – occurrence, mining, product of refining, Processing, color and constituency, classification and composition, grading of petroleum, determination of flash point, knocking, antiknock compounds, octane number, cetane number, chemical treatment to upgrade liquid fuel, Petrochemicals.

UNIT – IV **(9hrs.)**

Agrichemical Industries- Fertilizers – Fertilizer type, need for fertilizer, essential requirements, plant nutrients and regulators, soil fertility, pH of soil, classification of

fertilizer, natural fertilizers, nitrogenous fertilizer, Phosphate fertilizers, NPK fertilizers, effect of fertilizer- pollution. Insecticides- classification, DDT, BHC, Gammexane, Endosulfan. Attractant and repellants, fumigants, miticides, rhodenticide, fungicide, herbicide, acaricides. Pesiticide pollution- biological management, biodegradation, mode of poisoning, degradation and mobility.

UNIT – V **(12hrs.)**

Rubber Industries – Chlorinated and oxygenated rubber, latex, coagulation, crude natural rubber, vulcanization, physical and chemical properties. Synthetic rubbers- SBR, silicone rubber, reclaimed rubber, foam rubber, rubber cement, applications, Rubber derivatives. Leather – manufacture, tanning of leather – vegetable tanning, chrome tanning, oil tanning. Synthetic Fibers – properties, preparation, requirements, difference between synthetic and natural fiber. Rayon, Nylon, Orlon, Teflon.

Recommended Text Books:

1. C. A. Heaton, An Introduction to industrial chemistry, 2nd edition, 1991, Blackie.
2. George T. Austin, Shreve's Chemical Process Industries, 5th edition, 1984, McGraw Hill International.
3. B. K. Sharma, Industrial Chemistry (including Chemical Engineering), 1997, GOEL Publishing House.
4. M. Farhat Ali, Bassam El Ali, Handbook of Industrial Chemistry: Organic Chemicals, 2005, McGraw Hill Professional.
5. Fritz Ullmann, Ullmann's Encyclopedia of Industrial Chemistry, 1999-2014, John Wiley and Sons, Inc.
6. A. K. De, Environmental Chemistry, 7th edition, 2013, New Age International Publishers.
7. G. E. J. Poinern, A Laboratory Course in Nanoscience and Nanotechnology, 2015, CRC Press Taylor & Francis Group.

CHE 10606: Chemistry Lab – Physical **(2 credits, 64 hrs.)**

CST

Determination of mutual solubility of phenol-water system

Influence of KCl, Succinic acid on CST of phenol-water system-

Estimation of concentration of unknown solution

RAST METHOD

Determination of molal depression constant of naphthalene

Determination of molecular weight of solute

TRANSITION TEMPERATURE

Determination of transition temperature of salt hydrate-water system

Determination of molecular weight of solute

Viscosity, molecular weight of polymers

HALL EFFECT EXPERIMENT

Recommended Text Books:

1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan, 2014.
2. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. Laboratory Manual, CHE 10606, Department of Applied Chemistry, CUSAT

CHE10607 – Industrial Chemistry Lab **(2 credits, 64 hrs.)**

1. Preparation of soap and detergents
2. Preparation of margarine
3. Preparation and physical property measurement of natural, synthetic rubber, fiber.
4. Extraction of essential oils
5. Extraction of natural flavors
6. Preparation of Biogas
7. Waste water treatment
8. Preparation and characterization of nanomaterials
9. Preparation of silicon from Rice Husk

Recommended Text Books:

1. B. K. Sharma, Industrial Chemistry (including Chemical Engineering), GOEL Publishing House, 1997.
2. Fritz Ullmann, Ullmann's Encyclopedia of Industrial Chemistry, John Wiley and Sons, Inc, 1999-2014.
3. G. E. J. Poinern, A Laboratory Course in Nanoscience and Nanotechnology, CRC Press Taylor & Francis Group, 2015 .
4. Rohani AbuBakarab, RosiyahYahyaa, Seng NeonGan, Production of High Purity Amorphous Silica from Rice Husk, Procedia Chemistry, Volume 19, Pages 189-195, 2016.
5. Laboratory Manual, CHE 10607, Department of Applied Chemistry, CUSAT

CHE 10608: Open Ended Lab **(2 credits, 64 hrs.)**

CHE 10609: Computer Programming and Numerical Methods (2 credits, 32 hrs.)

UNIT – I (6 hrs.)

Programming in FORTRAN: Program design (algorithm), organization of program, data types and integer constants, complex constanta, logical constants, variables, implicit and explicit data typing, expressions and hierarchy of operations, mix-mode arithmatic, library functions, input/output specification, formatting, unconditional transfers, conditional statements and constructs, GO TO/ IF statements, relational operators, block if structure, else if construct, do loops, nesting, variables and arrays, parameter/data statements, common blocks, read/write by opening files, subroutines and construction of large program.

UNIT – II (5 hrs.)

Numerical Methods: Taylor's theorem, Expansion of functions, Remainder, Mean value and Extreme value theorems, Discrete average value theorem. Numerical Differentiation (first, second and higher derivatives)- Truncation and Round-off errors, Step size dilemma, Difference table (Pascal's triangle).

UNIT – III (5 hrs.)

Numerical Integration- Riemann sum, Quadrature rule, Interpolating polynomials (Lagrange's), Weights, Mid-point, Trapezoidal, Simpson's rule of integration, Adams' Predictor-Corrector method. Roots of equations- Newton-Raphson and Secant methods, Bisection and False-point methods, Bracketing method.

UNIT – IV (6 hrs.)

Numerical solution of ordinary differential equations- Initial value problems, Euler's method, Taylor and Runge-Kutta methods, Modified Euler and Hugen's method, Error estimates. Curve fitting- Least square fit algorithm, Monotone and convex data. Linear systems- Forward, Backward substitution, LU- factorization, pivoting (only basics), Gaussian Elimination, Gauss-Jordan Elimination, Jacobi and Gauss-Seidel methods. Eigenvalue problems. Statistical analysis of data.

UNIT – V (10 hrs.)

Programming Laboratory (Linux OS, vi editor): Students are instructed to write programs on some of the numerical methods taught. Programming in FORTRAN (FORTRAN 77 Standard)

Examples of numerical algorithms – algebraic equations, numerical integration, curve fitting, matrix computations

Text Books

1. M. Schatzman, Numerical Analysis: A Mathematical Introduction, 2nd Edn. Oxford University Press, 2012

2. J. M. McCormick and M. G. Salvadori, Numerical Methods in Fortran, Prentice Hall of India, 2009

3. R. L. Burden and J. D. Faires, Numerical Analysis, 2nd Edn. Brooks/Cole, 2012.

4. J. F. Epperson, An Introduction to Numerical Methods and Analysis, John Wiley and Sons, Inc., 2014

5. M. J. Maron, Numerical Analysis: A Practical Approach, , Macmillan, 2008.

6. F. B. Hildebrand, Introduction to Numerical Analysis, McGraw Hill, New York, 2007.

7. C. Xavier, Fortran 77 and Numerical Methods, 2nd Edn., New Age International Publishers, 2011

9. V. Rajaraman, Computer Programming in Frotran, PHI Learning, 1995.

10. S. A. Mollah, Numerical Analysis and Computational Programming, Allied Publishers (P) Ltd, 2011

CHE 10701: Quantum Chemistry **(3 credits, 48 hrs.)**

UNIT – I **(10 hours)**

Postulates of Quantum Mechanics. Time dependent and time independent Schrodinger wave equation. Conservative systems, Stationary states, Formulation of quantum mechanical problems, Application of Schrodinger wave equation for particle in one dimensional box, Particle in two and three dimensions.

UNIT – II **(10 hrs.)**

Separation of variables, concept of degeneracy, Introduction to quantum mechanical tunnelling. Vibrational motion, Harmonic oscillator, Method of power series, Hermite equation and Hermite Polynomials, Recursion formula, Rodrigues formula, wave function and energy. Rigid rotator, Wave function in spherical polar coordinates, Planar rotator, phi equation, wave functions in real forms, Polar diagrams, Nonplanar rotator, Theta equation and solutions Lagendre equation and Lagendre polynomials, Spherical harmonics, Angular momentum operator L2 and Lz, Space quantization.

UNIT - III **(8 hrs.)**

H atom, the R equation, Laguerre equation and Laguerre polynomials wave equation and energy of H like systems, Radial function and radial distribution functions, Shapes of s, p, d and f atomic orbitals.

UNIT -IV **(10 hrs.)**

Postulate of electron spin - orbital and spin functions. Many electron atoms. Approximation methods: Variation theorem and its proof, application to particle in one dimensional box, Helium atom. Perturbation method, First order perturbation, Application to helium atom. Term symbols for atoms. Hartree Fock Self Consistent Field method, Slater's treatment of complex atoms, Slater orbitals. Pauli principle, Slater determinant and wave function.

UNIT – V **(10 hrs.)**

Born Oppenheimer approximation, MO theory for the ground state and excited state of H_2^+, hydrogen molecule - MO treatment and calculation of energy, molecular term symbols, Molecular orbital method for diatomic molecules, Correlation diagram, Non-crossing rule. Valence bond method. H_2^+ and H_2 molecule, Comparison of VB and MO method, Bonding in simple molecules like water, BF_3, NH_3, CH_4, VSEPR theory, Pi bonding in simple molecules. HMO method for linear conjugated hydrocarbons, aromatic hydrocarbons, calculation of free valence charge density and reactivity.

Recommended Text Books:

1. Griffiths, D. J. Introduction to Quantum Mechanics, 2nd Ed., Cambridge University Press, 2016.
2. Atkins, P. W. and Friedman, R. S. Molecular Quantum Mechanics, 5th Ed., Oxford University Press, New York, 2010.
3. Mc Quarrie, D. A. Quantum Chemistry, 2nd Ed., University Science Books, 2007.
4. Prasad, R. K. Quantum Chemistry, 4th Ed., New Age Science, 2009.
5. Levine, I. N. Quantum Chemistry, 7th Ed., Pearson, 2013.
6. Lowe, J. P. and Peterson, K. Quantum Chemistry, 3rd Ed., Academic Press, 2005.

CHE 10702: Structural Inorganic Chemistry of Main Group (3 credits, 48 hrs.)

UNIT – I (12 hrs.)

Structure and bonding in polyhedral boranes and carboranes, styx notation; electron count in polyhedral boranes; Wade's rule; topological approach to boron hydride structure. Styx numbers. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures. synthesis of polyhedral boranes; mno rule, Carboranes Metallocarboranes. boron halides; phosphine-boranes; boron heterocycles; borazine, borophenes.

UNIT – II (8 hrs.)

Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. SxNy compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}. Phosphorus-nitrogen compounds: Phosphazenes. Cyclo and linear phosphazenes.

UNIT – III (8 hrs.)

Silanes, silicon halides, silicates, silicones, silanols; germanium, tin and lead organyls; silenes, germenes and stannenes; fullerenes; carbon nanotubes (CNT's) and graphenes, silicon carbides.

UNIT -IV (8 hrs.)

Relative strength of acids, Pauling rules, Lux-Flood concept, Lewis concept, Measurement of acid base strength sytematics of Lewis acid –base interactions steric and salvation effects acid –base anomalies, Pearson's HSAB concept, acid-base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness. Chemistry in non aqueous solvents reactions in NH_3, liquid SO_2, solvent character, reactions in SO_2, acetic acid, solvent character, reactions in CH_3COOH and some other solvents. Molten salts as non aqueous solvents solvent properties room temperature molten salts. unreactivity of molten salts, solutions of metals.

UNIT -V (12 hrs.)

Macrocycles and supramolecules non-covalent forces and interactions in supramolecules,:crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils, self-assembly and preorganization, coordination driven self-assembly of supramolecular two and three dimensional architectures, host-guest chemistry, CO_2 capture, metal-organic frameworks and their applications, zeolites and its application in catalysis.

Recommended Text Books:

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, and M. Bochmann Advanced Inorganic Chemistry, 6th Ed., Wiley-Interscience: New York, 1999.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L. Inorganic Chemistry, Principle and structure and reactivity, 4th Ed., Harper Collins College Publishers, New York, 1993.
3. Steed, J. W. and Atwood, J. L. Supramolecular Chemistry, 2nd Ed., John Wiley & Sons Ltd., 2009.
4. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
5. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, 3rd Ed., Oxford, 1994.
6. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, 2nd., Ed. Butterworth-Heinemann,1997.
7. Lehn, J. M., Supramolecular Chemistry: Concepts and Perspectives, Wiely VCH, 2006.

CHE 10703: Statistical and Equilibrium Thermodynamics (3 credits, 48 hrs.)

UNIT – I (9 hours)

Types of Molecular velocities- derivation and calculation, Maxwell's distribution of molecular velocities, Effect of temperature on distribution, Transport properties- Diffusion, effusion, Viscosity, Thermal conductivity.

Thermodynamic probability, microstate and macrostate, entropy and probability, most probable distribution, residual entropy and its calculation. Ensembles, Maxwell - Boltzman statistics.

UNIT – II (10 hours)

Partition function and its relation to thermodynamic properties, Translational, rotational and Vibrational partition function. Molecular partition function for delocalized systems, calculation of equilibrium constant using partition functions. Heat capacity of gases, Anomalous heat capacity of H_2, Heat capacity of solids: Dulong - Petits law, Einstein's theory and its modification, Debye's theory of heat capacity of solids.

UNIT - III (10 hours)

Quantum statistics, Bose - Einstein statistics, Fermi - Dirac statistics, Comparison of Maxell - Boltzman, Bose=- Einstein and Fermi - Dirac Statistics, Dilute Systems. Application of Bose -Einstein Statistics, Gas degeneration, Application to liquid helium, Bose Einstein Condensation. Application of Fermi -Dirac Statistics to electrons in metals, Extreme Gas Degeneration, Electron gas in metals and its contribution to pressure and heat capacity.

UNIT – IV (9 hours)

Partition function for systems of dependent particles, Configurational integral and configurational partition function. Imperfect gas, Van der waals equation and Virial equation of state, Evaluation of the first virial coefficient. Condensed state, Cluster integrals, Communal entropy.

UNIT - V (10 hours)

Linear Non-equilibrium thermodynamics- General theory, Local entropy production, balance equation for concentration. Energy conservation in open systems. Entropy balance equation. Forces and Fluxes, Steady state and local equilibrium conditions. Linear phenomenological laws. Phenomenological coefficient, Systems with heat, matter and electrical transport, Onsager Reciprocal relation, Application to Diffusion -Thermal diffusion, Thermal Osmosis and electrokinetic effects, Soret Coefficient, Seebeck effect.

Recommended Text Books:

1.F.W. Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub.,1 3rd edn, 1978,.

2. F.C. Andrews, Equilibrium to Statistical Mechanics, John Wiley,2nd edn, 1975.

3. Malcolm Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London.

4. L.K. Nash, Statistical Thermodynamics, Addison Wesley,1967.

5. J. Kestin and J.R. Dorfman, A course in Statistical Thermodynamics, Academic press, 1971.

6. D. Kondepudi and I. Prigogine, Modern Thermodynamics: From Heat Engines to Dissipative Structures, Wiley, New York.

CHE 10704: Stereochemistry **(3 credits, 48 hrs.)**

UNIT – I **(9 hrs)**

Geometrical & Optical isomerism: origin of chirality, chiral centres, axes and planes, helicity, enantiotopic and diastereotopic, groups and faces, prochiral centres and faces, allenes, cumulenes, biphenyls, and spirans. Compounds containing chiral atoms other than carbon.

UNIT – II **(10 hrs)**

Conformational analysis: small and medium rings with special emphasis on mono and disubstituted six membered rings, bicyclic systems. Conformation and Stereo-electronic Effects of carbohydrates: D and L sugars, Chair conformation, Endo/Exo-anomeric effect, Reverse anomeric effect, Glycosidic torsion angles, Hydroxymethyl group conformation. Conformation and stability of aldohexoses, structure and conformation of ribose and deoxyribose.

UNIT – III **(10 hrs)**

Reaction Mechanisms and Conformational Effects on Reactivity - Ester Hydrolysis, Alcohol Oxidations, S_N2 Reactions, Elimination Reactions, Epoxidation by Intramolecular closure of Halohydrins, Epoxide Openings (S_N2), Electrophilic Additions to Olefins, Rearrangement Reactions, Conformational and Stereoelectronic Effects on Reactivity. Baldwins rules for ring closure.

UNIT – IV **(10 hrs)**

Stereoselective Nucleophilic Additions to Acyclic Carbonyl Groups. Cram's Rule. Felkin-Ahn Model. Effect of Chelation on Selectivity. Diastereoselectivity in Aldol Reactions. Stereoselective Reactions of Acyclic Alkenes. The Houk Model.

UNIT – V **(9 hrs)**

Stereoselective Reactions of cyclic compounds. Reactions on Small Rings. Stereochemical Control in Six Membered Rings. Stereochemistry of Bicyclic Compounds. Reactions with Cyclic Intermediates/Transition states.

Recommended Text Books:

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Ed., Wiley, 2013.
2. Lowry, T H. and Richardson, K.S. Mechanism and Theory in Organic Chemistry, 3rd Ed., Benjamin-Cummings Publishing Company, 1997.
3. Carey, F. A. and Sundberg, R. J., Advanced Organic Chemistry (parts A and B), 5th Ed., Springer, 2008.
4. Anslyn, E.V. and Dougherty, D.A. Modern Physical Organic Chemistry. University Science Books, 2005.
5. Carroll, F.A. Perspectives on structure and mechanism in organic chemistry, 2nd Ed., Wiley, 2010.
6. Issacs, N. S. Physical Organic Chemistry, Second Edition, 2nd Ed., Prentice Hall, 1995.
7. Pross, A. Theoretical and Physical Principles of Organic Chemistry, 1st Ed., Wiley, 1995.
8. Clayden, J. Green, N. Warren, S. and Wothers, P. Organic Chemistry, 2nd Ed., Oxford University Press, 2012.
9. Kalsi, P.S. Stereochemistry, Conformation and Mechanism, 8th Ed., New Age Publications, 2014.
10. Eliel, E. L. and Wilen, S. H. Stereochemistry in Organic Compounds, Student Ed., John Wiley, 2008.
11. Pine, S. H. Organic Chemistry, 5th Ed., McGraw Hill, 2008.
12. Flemming, I. Molecular orbitals and organic chemical reactions, student edition, Wiley 2009.
13. McMurry, J. Organic Chemistry, 5th Edition, Brooks/Cole, 2000.
14. Nasipuri, D. Stereochemistry of Organic Compounds: Principles and Applications, 3rd Ed., New Age, 2018.

CHE 10705: Organic Photochemistry, Pericyclic Reactions and Rearrangements

(3 credits, 48 hrs.)

UNIT – I **(9 hrs)**

Pericyclic reactions: study of the principle of conservation of orbital symmetry, Orbital symmetry diagrams for cycloaddition and electrocyclic reactions, Orbital Correlation diagram, Study of Frontier Molecular Orbital Theory, Aromatic Transition State Theory and The Generalized Woodward – Hoffmann rule applied to cycloaddtions, electrocyclic reactions, [i, j] sigmatropic rearrangements and chelotropic reactions.

UNIT – II **(9 hrs)**

Stereochemistry and regiochemistry of cycloadditions. Substituent and medium effects, secondary orbital interactions in [4+2] cycloadditions Intramolecular Diels–Alder reactions. 1,3-dipolar cycloaddition reactions. Photochromism and thermochromism, sigmatropic rearrangements, Cheletropic fragmentation and ene-reaction. Applications in organic synthesis.

UNIT – III **(9 hrs)**

Photochemistry: Electronic transitions in organic molecules. Laws of photochemistry, singlet and triplet excited, Fate of photoexcited molecules, Jablonski diagram– unimolecular photophysical processes – fluorescence, phosphorescence, delayed fluorescence, bimolecular – sensitization and quenching, excited state energy and electron transfer.

UNIT – IV **(9 hrs)**

Types of photochemical reactions, photochemistry of carbonyl compounds and alkenes – photoreduction, photocycloaddition, *cis-trans* isomerization, photodimerization, photo induced electron transfer, rearrangements in the excited state. Valence isomerization, photosubstitution reactions, mechanism of important photochemical reactions - Paterno-Buchi reaction, Norrish Type I and Type II fragmentation, Barton reaction, photochemistry of arenes and nitrocompounds., singlet oxygen, chemi and bioluminescence. Chemistry of vision

UNIT – V **(12 hrs)**

Rearrangements in the ground and excited state: Rearrangements involving electron deficient carbon and nitrogen. Mechanism of the following rearrangements: Wagner-Meerwein, Pinacol, Demjanov, dienone-phenol, benzilic acid, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, benzidine, and Hofmann-Loffler rearrangements. Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Seyferth-Gilbert homologation, Grubbs catalysts and olefin metathesis. Di-Π methane, cycclohexadienone photochemistry, Fries and photoFries rearrangement

Recommended Text Books:

1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Ed., Wiley, 2013.
2. Lowry, T H. and Richardson, K.S. Mechanism and Theory in Organic Chemistry, 3rd Ed., Benjamin-Cummings Publishing Company, 1997.
3. Carey, F. A. and Sundberg, R. J., Advanced Organic Chemistry (parts A and B), 5th Ed., Springer, 2008.
4. Anslyn, E.V. and Dougherty, D.A. Modern Physical Organic Chemistry. University Science Books, 2005.
5. Issacs, N. S. Physical Organic Chemistry, Second Edition, 2nd Ed., Prentice Hall, 1995.
6. Pross, A. Theoretical and Physical Principles of Organic Chemistry, 1st Ed., Wiley, 1995.
7. Clayden, J. Green, N. Warren, S. and Wothers, P. Organic Chemistry, 2nd Ed., Oxford University Press, 2012.
8. Flemming, I. Frontier orbitals and organic chemical reactions, Wiley-Blackwell, 1976.
9. Flemming, I. Molecular orbitals and organic chemical reactions, student edition, Wiley 2009.
10. McMurry, J. Organic Chemistry, 5th Edition, Brooks/Cole, 2000.

11. Bruckner, R. Advanced organic chemistry: Reaction Mechanisms, 1st Ed., Academic Press, 2001.
12. Norman, R.O.C. Principles of Organic Synthesis, 2nd Ed., Chapman and Hall, 1978.

CHE 10706: Chemistry Lab – Physical **(2 credits, 64 hrs.)**

PHASE DIAGRAM

Construction of phase diagram of Naphthalene-Biphenyl, Naphthalene-Diphenyl amine systems and determination of unknown composition

Three component system involving three liquids- Construction of phase diagram and determination of unknown composition

PARTITION

Study of the distribution of I_2 between water/$CHCl_3$ or toluene, benzoic acid/succinic acid between toluene and water

Determination of equilibrium constant of $I_2 + KI \leftrightarrow KI_3$

DETERMINATION OF CMC

ADSORPTION

Adsorption of acetic acid/ oxalic acid on charcoal- verification of Langmuir and Freundlich isotherms

KINETICS- SINGLE, DOUBLE KINETICS

Rate constant for ethyl acetate hydrolysis catalyzed by HCl

Rate constant for ethyl acetate hydrolysis catalyzed by NaOH

Recommended Text Books:

1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan, 2014.
2. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. Laboratory Manual, CHE 10706, Department of Applied Chemistry, CUSAT

CHE 10707: Organic Chemistry Lab (Estimation and Separation)

(2 credits, 64 hrs.)

Estimation of organic compounds

Separation of Organic binary mixtures – steam distillation, column chromatography, liquid-liquid extraction.

Recommended Text Books:

1. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2nd Ed., 2007.
2. Dey, B.B. Sitaraman, M.V. and Govindachari, T.V. Laboratory Manual of Organic Chemistry, 3rd Ed., Viswanathan, 1957.
3. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Longman, 1989.
4. Mann, F.G. Saunders, B.C. Practical Organic Chemistry, 4th Ed., Pearson Education India, 2009.
5. Clark, H.T. A handbook of organic analysis, Longman, 1966.
6. Laboratory Manual, CHE 10707, Department of Applied Chemistry, CUSAT.

CHE 10708: Open Ended Lab **(2 credits, 64 hrs.)**

CHE 10709: Chemistry of Polymers **(2 credits, 32 hrs.)**

UNIT – I **(6 hrs.)**

History of Polymer Science. Concept of macromolecules, Principle of duality, Integration of molecular character and material character. Molecular design, synthesis and process technologies. Nomenclature and Classification. Raw Material sources of polymers. Natural gas, coal and petroleum. Monomers and polymers derived from natural gas. Petroleum and petrochemicals. Monomers and polymers derived from ethylene and propylene. Monomers and polymers derived from C4 and C5 Systems and BTX fraction. Acetylene as a source of monomers.

UNIT – II **(8 hrs.)**

Polymerization processes. Free radical addition polymerization. Kinetics and mechanism. Chain transfer. Molecular weight distribution and molecular weight control. Cationic and anionic polymerization. Polymerization without termination. Living polymers. Step Growth polymerization. Kinetics and mechanism. Linear Vs cyclic polymerization, Group Transfer, metathesis and ring opening polymerization. Copolymerization. The copolymerization equation, Q-e scheme, Gelation and Crosslinking. Copolymer composition drift. Polymerization techniques. Bulk Solution, melt, suspension, emulsion and dispersion techniques.

UNIT – III **(6 hrs.)**

Polymer Stereochemistry. Organizational features of polymer chains. Configuration and conformation, Tacticity, Repeating units with more than one asymmetric center. Chiral polymers – main chain and side chain. Stereoregular polymers. Manipulation of polymerization processes. Zeigler-Natta and Kaminsky routes. Coordination polymerization. Metallocene and Metal oxide catalysts.

UNIT – IV **(6 hrs.)**

Polymer Characterization. Molecular weights. Concept of average molecular weights, Determination of molecular weights. GPC and Light scattering techniques. Molecular weight distribution. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition

and crystalline melting. Spherullites and Lammellae. Degree of Crystallinity, Thermal analysis of polymers. TG/DTG, DTA/DSC, Spectroscopy of polymers. Microstructure determination by IR, Raman, UV, NMR and MS techniques. Solid State NMR and polymer stereochemistry.

UNIT – V **(6 hrs.)**

Industrial polymers. Synthesis, Structure and applications. Polyethylene, polypropylene, polystyrene. PVC, PVA, PAN, PA. Poly(vinyl carbazole), poly(vinyl imidazole). PMMA and related polymers. Flourine containing polymers. Reaction polymers. Polyamides, polyesters. Epoxides, polyurethanes, polycarbonates, phenolics, PEEK, Silicone polymers. Reactions of polymers. Polymers as aids in Organic Synthesis. Polymeric Reagents, Catalysts, Substrates, Liquid Crystalline polymers. Main chain and side chain liquid crystalline polymers.

Recommended Text Books:

1. Billmayer, F.W. Textbook of Polymer Science. 3rd Ed., Wiley. N.Y. 1991.
2. Cowie, J.M.G. Polymers: Physics and Chemistry of Modern Materials. Blackie. London, 1992.
3. Young, R.J. Principles of Polymer Science, 3rd Ed., Chapman and Hall. N.Y. 1991.
4. Flory, P.J. A Text Book of Polymer Science. Cornell University Press. Ithacka, 1953.
5. Ullrich, F. Industrial Polymers, Kluwer, N.Y. 1993.
6. Elias, H.G. Macromolecules, Vol. I & II, Academic, N.Y. 1991.
7. Brydson, J.A. Polymer chemistry of Plastics and Rubbers, ILIFFE Books Ltd., London, 1966.

CHE 10710: Materials Chemistry **(2 credits, 32 hrs.)**

UNIT – I **(6 hrs.)**

Chemistry of Materials. Historical perspectives – strategies for the design of new materials-a critical thinking approach. Ionic and covalent solids. Molecular and metallic solids. Amorphous and crystalline materials. Crystalline state. Structural organization of crystalline solids-theories of bonding. Crystal structures. Imperfections in crystal structures. Amorphous materials – glasses and ceramic solids. Structural organization of amorphous solids. Traditional ceramics. Synthetic high performance ceramics. Crystal structure of ceramics.

UNIT – II **(6 hrs.)**

Metals and alloys. Structural and bonding theories of metals. Alloys -ferrous alloys – phase behavior of ferrous alloys. Behaviour of binary alloys. Intermediate compounds and intermediate phases. Nonferrous metals and alloys. Shape memory alloys. PZT materials. Optical, electrical and magnetic properties of metallic materials.

UNIT – III **(6 hrs.)**

Semiconductor materials- properties and types of semiconductors. Structure and Bonding of semiconductor materials. Silicon based semiconductors. II-VI (wide band gap) and IIIV (narrow band gap) compound semiconductors. Electrical, optical and magnetic properties of semiconductor materials. Preparation and properties of ZnO, ZnS, CdS, CdTe, Ga-As, In-S, Cu-In-S. Application in photovoltaic devices

UNIT – IV **(8 hrs.)**

Polymer Materials- classification and nomenclature of polymers. Methods of Polymerization. Dendritic and cascade polymers. Polymers via Click Chemistry. Properties of polymers. Plastics and elstomers. Viscoelastic behavior. Rubber like elasticity. Crystalline and amorphous polymers. Glass transition temperature and crystalline melting. Polymer composites- polymer matrix composites.

Nanomaterials. Materials in the nanodomain. Zero, one and two dimensional materials. Particle size dependent change in properties of materials. Metals in the nanodomain. Gold

and silver nanoparticles. Preparation, properties and applications. Core shell structures. Semiconductor nanoparticles. Quantum dots. ZnO, ZnS, CdS and CdSe quantum dots. Electrical and optical properties. Nano domains of Carbon-fullerenes, carbon nanostructures, graphene.

UNIT – V **(6 hrs.)**

Characterization of Materials. Optical Microscopy- Principles, instrumentation and application of confocal raman microscopy, SPM/STM. Electron microscopy- SEM, FESEM, TEM. Principles, instrumentation and applications. Surface and core level techniques- Photoelectron spectroscopy- X-Ray and UV. Thermal methods- TG/DTG, DTA, DSC, DMA. X-Ray Diffraction

Recommended Text Books:

1. Fahlman, B. D. Materials Chemistry, 2nd Ed., Springer, Heidelberg, 2011.

2. Zallen, R. Physics of Amorphous Solids, Wiley, New York, 1983.

3. Borg, R. J. and Dienes, G. J. The Physical Chemistry of Solids, Academic Press, Boston, 1993.

4. Kingery, D.; Bowen, H. K.; Uhlmann, D. R. Introduction to Ceramics, 2nd Ed., Wiley, New York, 1992.

5. Cowie, J. M. J. Polymers. Physics and Chemistry of Modern Materials, 3rd Ed., CRC Press, Boca Raton, 2007.

6. Kasap, S. O. Principles of Electronic Materials and Devises, Mc Graw Hill,2006.

CHE 10711: Advanced Equilibrium Thermodynamics (2 credits, 32 hrs.)

UNIT – I (6 hrs.)

Mathematical techniques: Variables of thermodynamics, theoretical methods, Practical techniques. First law of thermodynamics, thermodynamic functions, heat capacity, thermochemistry. Joule Thomson effect. Coefficient of thermal expansion and compressibility factor.

UNIT – II (8 hrs.)

Second law of thermodynamics. Entropy. The Clausius inequality. Entropy changes accompanying expansion, phase transition and heating. free energy functions. Third law of thermodynamics: Need for third law Calculation of absolute entropy, unattainability of absolute zero. Relation between thermo dynamic functions. Maxwell relations. Variation of entropy with temperature and pressure.

UNIT – III (6 hrs.)

Thermodynamic systems of variable composition. Fugacity functions. Partial molar quantities; Gibbs-Duhem equations. Duhem-Margules equations. Henry's law, Rault's law. Thermodynamics of ideal solutions, real solutionand regular solutions. Dilute solutions of nonelectrolytes, Activity and standard states of nonelectrolytes,

UNIT – IV (6 hrs.)

Phase rule – Application to one, two and three component systems. Liquid-vapour equilibria of binary systems.

UNIT – V (6 hrs.)

Applications of free energy function to physical and chemical charges. Equilibrium in chemical reactions. Effect of temperature and pressure on chemical equilibrium- Van't Hoff reaction isochore and isotherm

Recommended Text Books:

1. Atkins, P. and Paula, J. de Physical Chemistry, 7th Ed., or later editions, W. H. Freeman and Company, New York. 2006.
2. Klotz, I.M. and Robsenberg, R.M. Chemical Thermodynamics, 3rd Ed., W.A.Benjamin, INC.1972.
3. Nash, L.K. Elements of Chemical Thermodynamics, Addison Wesley. Prigogine, Introduction to thermodynamic irreversible processes, Interscience. 1962.

CHE 10712: Environmental Chemistry **(2 credits, 32 hrs.)**

UNIT – I **(6 hrs.)**

Global warming – Ozone hole. Environmental segments – The hydrological cycle – The oxygen cycle – The nitrogen cycle – The sulphur cycle – Composition of atmosphere – Earth's radiation balance – Green house effect.

UNIT – II **(6 hrs.)**

Air pollution – Primary pollutants, Acid rain – Air quality standards – Sampling – Monitoring – Analysis of CO, nitrogen oxides, sulphur oxides, hydrocarbons and particulate matter – Control of air pollution.

UNIT – III **(6 hrs.)**

Soil pollution – Inorganic and organic components in soil – Acid – Base and ion exchange reactions in soils – Micro and macro nutrients – Wastes and pollutants in soil.

UNIT – IV **(8 hrs.)**

Water pollution – Water pollutants – Eutrophication – Water quality criteria for domestic and industrial uses – Trace elements in water – Determination of quality parameters – Total hardness, TDS, pH, chloride, heavy metals, etc.

Principles of water and waste water treatment – Aerobic and anaerobic treatment – Industrial waste water treatment – Removal of organic and inorganic materials from water and waste water.

UNIT – V **(6 hrs.)**

Instrumental techniques in environmental analysis – Use of neutron activation analysis – ASV, AAS, GC, HPLC, ion selective electrodes and ion chromatography in environmental chemical analysis.

Recommended Text Books:

1. Environmental Chemistry , Gary W. VanLoon, Stephen J. Duffy, Oxford University Press, 2005

2. Principles Of Environmental Chemistry, James Girard, Jones & Bartlett Learning, 2005

3. Environmental Chemistry, Seventh Edition, Stanley E. Manahan, CRC Press, 2010

4. Applications of Environmental Chemistry, Eugene R. Weiner, CRC Press,2010

5. Environmental chemistry, Ian Williams, J. Wiley, 2001

6. The essential guide to environmental chemistry, Georg Schwedt, John Wiley, 2001

CHE 10713: Biomolecules and Bioorganic Chemistry **(2 credits, 32 hrs.)**

UNIT – I **(6 hrs.)**

Carbohydrates. Structure and biological function - monosaccharides, disaccharides, polysaccharides – storage form of cell fuel, structural and protective polysaccharides, glycoproteins, mucopolysaccharides and proteoglycans. Glycolysis and Citric acid cycle.

UNIT – II **(8 hrs.)**

Amino acids, Peptides and Proteins - Classification and nomenclature of amino acids – stereochemistry of amino acids, properties of amino acids—isoelectric points - Protein structure – determination of primary structure – end terminal analysis – secondary, Tertiary structure and structural motifs-protein folding and domain structure of proteins. Quaternary structure of proteins. Purification and characterization of proteins. Fibrous protein – α-Keratin, β-Keratin, collagen, Globular proteins – properties and function. Myoglobin and Hemoglobin – oxygen binding curves.

UNIT – III **(6 hrs.)**

Enzymes, Coenzymes and Vitamins. Classification, specificity of enzyme action, Reversible inhibitors – competitive and noncompetitive, Isoenzymes. Allosteric enzymes. Coenzymes-function of coenzyme, mechanism of action of metalloenzyme, Classification and function of vitamins, mechanism of action of coenzymes. Role of inorganic elements in biological function.

UNIT – IV **(4 hrs.)**

Lipids Fatty acids, waxes, fats and oils, Phospholipids and cell membranes, Biosynthesis of fatty acids.

UNIT – V **(8 hrs.)**

Nucleic Acid. Nucleosides and nucleotides, ATP - carrier of chemical energy, mechanism for phosphoryl transfer reactions, nucleic acids - helical forms of DNA, Replication and transcription of DNA.

Recommended Text Books:

1. Voet, D. and Voet, J. G. Biochemistry, 4th Ed., John Wiley, 2010.

2. Nelson, D.L. and Cox, M.M. Lehninger Principles of Biochemistry, 5th Ed., W. H. Freeman and CBS Publishers, 2008.
3. Berg, J. M. Tymoczko, J. L. and Stryer, L. Biochemistry, 5th Ed., W. H. Freeman, 2002.
4. Finar, I. L. Organic Chemistry Volumes 1 & 2, 6th Ed., Pearson Education Asia, 2004.
5. Krishnaswamy, N. R. Chemistry of Natural Products; A Unified Approach, 2nd Ed., Universities Press, 2010.
6. Simmonds, R. J. Chemistry of Biomolecules: An Introduction, RSC, 1992.
7. Morrison, R.T. Boyd, R.N. and Bhattacharjee, S.K. Organic Chemistry, 6th Ed., Pearson Education Inc., 2014.
8. Bruice, P.Y. Organic Chemistry, 7th Ed., Prentice Hall Inc., 2013.
9. Smith, M. B. Organic Synthesis, 2nd Edition, McGraw-Hill, 2000.

CHE 10801: Group Theory and Spectroscopy **(3 credits, 48 hrs.)**

UNIT – I **(8 hours)**

Molecular symmetry: Symmetry elements and operations, Point groups, Matrix representation of symmetry operations, character, Application of Group theory to symmetry properties of molecules, Definition of a mathematical group, Abelian group, cyclic group, symmetry operations as group elements, similarity transformation and classes Group multiplication table – Symmetry classification of molecules into point groups (Schoenflies symbol)- Application of symmetry to predict polar and chiral compounds.

UNIT – II **(10 hrs.)**

Reducible and Irreducible representations - Great Orthogonality theorem and its consequences, Character tables- reduction formula- Construction of character tables for point groups Interpretation of character tables. Mülliken symbols, reduction formula, direct sum and direct products. Wave functions as bases for irreducible representations, Construction of hybrid orbitals for AB_3(planar), AB_4(Td), AB_5(D_{3h}) and AB_6(Oh) type of molecules - Symmetry adapted linear combinations, Projection operators, Application of projection operators to pi-bonding in ethylene, cyclopropenyl systems and benzene.

UNIT – III **(10 hours)**

Interaction of electromagnetic radiation with matter: Electromagnetic radiation, radiation density, Energy levels in molecules, Absorption and emission of radiation, Intensity and width of spectral lines, Beer lambert's law, Integrated absorption coefficient, Line width – natural line broadening, Doppler broadening, minimisation of line broadening, Induced and spontaneous transitions, correlation to the Einstein coefficients of absorption and emission, Basis of selection rules Fermi golden rule, lasers, Spectroscopy and quantum mechanics, Born-Oppenheimer approximation.

UNIT – IV **(10 hours)**

Rotational spectroscopy: Rotation of rigid bodies, moment of inertia, linear molecules, spherical, symmetric and asymmetric tops, selection rules, rotational spectra and line intensities, structure determination from rotational constants, isotopic effects.

Vibrational Spectroscopy: Review of vibrational motion in diatomics, vibrational selection rules, dissociation energies, vibration-rotation transitions in diatomics, harmonic oscillator, anharmonicity, centrifugal distortion, Vibration of polyatomic molecules, normal modes, combination, difference and hot bands, Fermi Resonance, group theoretical treatment of vibrations.

Raman Spectroscopy: Review of light scattering and Raman effect, classical and quantum models for scattering, polarizability, selection rules, group theoretical treatment of vibrations. mutual exclusion rule for centrosymmetric molecules, polarized and depolarized Raman lines, resonance Raman scattering.

Electronic Spectroscopy of molecules: Molecular orbitals and states, term symbols,selection rules, vibrational and rotational structures, Frank-Condon principle, photoelectron spectroscopy, dissociation and predissociation, calculation of heat of dissociation, Birge Sponer method, electronic spectroscopy of polyatomic molecules, UPES and XPES

UNIT – V **(10 hours)**

NMR & EPR: Expression for Hamiltonian/Energy - Zeeman interaction, torque exerted by a magnetic field on spins, equation, its solution and the physical picture of precession. Thermal equilibrium, Relaxation, chemical shift, shielding and deshielding, Karplus relationships,Bloch equations, the rotating frame, pulsed experiments, NOE, double irradiation, selective decoupling, double resonance, Polarisation transfer, Two dimensional NMR, Solid state NMR, NQR, MRI

EPR Hamiltonian, g factor, hyperfine interactions, Kramer's degeneracy

Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum,chemical shift, factors determining chemical shift, application to metal complexes, Mossbauer spectra of Fe(II) and Fe(III) cyanides.

Recommended Text Books:

1. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern, Singapore, 2nd Ed., 1992.

2. V. Ramakrishnan & M. S. Gopinadhan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996

3. P. W. Atkins, Physical Chemistry 8th Ed. W. H. Freeman, New York, 2006

4. R. A. Alberty, Physical Chemistry 8th Ed., Wiley, New York., 1994

5. I. N. Levine, Molecular Spectroscopy, John Wiley & Sons.

6. J. M. Hollas, Modern Spectroscopy, John Wiley & Sons.

7. P. F. Bernath, Spectra of Atoms and Molecules, III Edn, Oxford University Press.

8. J. L. McHale Molecular Spectroscopy, Pearson Education.

9. W. W. Parson, Modern Optical Spectroscopy, Springer-Verlag.

10. Jack D. Graybeal, Molecular Spectroscopy, Mc Graw Hill International Editions

11. M.H. Levitt, Spin Dynamics, II edn.Wiley

12. James Keeler, Understanding NMR spectroscopy, II edn. Wiley

13. Harald Gunther, NMR spectroscopy: Basic principles, Concepts and Applications in chemistry, 3rd edn

14. Russell S Draggo, Physical methods in inorganic chemistry, II Edn., 1977.

CHE 10802: Chemistry of Transition metals **(3 credits, 48 hrs.)**

UNIT – I **(10 hrs.)**

Splitting of d orbitals in different crystal fields such as octahedral, tetragonal, square planar, tetrahedral, trigonal bipramidal and square pyramidal fields. Energy levels of d orbitals in crystal fields of different symmetries crystal field stabilization energy and its calculations. Thermodynamic effects of LFSE. Factors affecting the splitting parameter. Spectrochemical series. Molecular orbital theory based on group theoretical approach and bonding in metal complexes. σ and π bondings in complexes. MO diagrams of complexes with and without π bonds. Effect of π bond on the stability of σ bond. Nephelauxetic series.

UNIT – II **(10 hrs.)**

Electronic Spectra of complexes: Term symbols of dn system, Raccah parameters, splitting of terms in weak and strong octahedral fields. Correlation diagrams for dn and d10-n ions in octahedral and tetrahedral fields (qualitative approach), d-d transition, selection rules- effect of spin-orbit coupling Orgel diagrams- splittings for d^1, d^9 and high spin d^4 and d^6, splittings for d^2, d^3, d^8 and high spin d^7 (ii) Tanabe-Sugano diagrams- spectra of d^7, d^5 and low spin d^6 complexes. Calculation of Dq, B and β (Neplauxetic ratio) values. Spectra of complexes with lower symmetries. Jahn Teller effect and its consequences on the nature of the electronic spectra. Charge transfer spectra electronic spectra of lanthanide and actinide complexes

UNIT – III **(8 hrs.)**

Types of magnetic behaviour, magnetic susceptibilities, Pascal's constants, paramagnetism in experimental simple systems where S = ½, van Vleck's equation, its derivation and its applications. Spin-orbit coupling and susceptibility of transition metal ions and rare earths; magnetic moments of metal complexes with crystal field terms of A, E and T symmetry, intramolecular effects, antiferromagnetism and ferromagnetism of metal complexes, super paramagnetism. High and low spin equilibria. Magnetic properties of lanthanides and actinides

UNIT – IV **(10 hrs.)**

Electronic paramagnetic resonance spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. EPR spectrometers, presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Second order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

UNIT – V **(10 hrs.)**

Thermodynamic and kinetic stability. Kinetics and mechanism of nucleophilic substitution reactions in square planar complexes. Mechanism of entering and other leaving groups and trans effect. Kinetics and mechanism of octahedral substitution, - Dissociative and associative mechanisms, base hydrolysis, Racemization reactions, Trans effect, trans effect series, and theories of trans effect Electron transfer reactions-outer sphere mechanism-Marcus theory, inner sphere mechanism.

Recommended Text Books:

1. F. A. Cotton, G. Wilkinson, C. A, Murillo, and M. Bochmann Advanced Inorganic Chemistry, 6th Ed., Wiley-Interscience: New York, 1999.
2. J.E. Huheey, Ellen A. Keiter and Richard L. Keiter, Inorganic Chemistry, Principles of structure and Reactivity, 4th Ed., Harper Collin College Publishers, 1993.
3. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, 2nd Ed., John Wiley & Sons Ltd., 2009.
4. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
5. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, 3rd Ed., Oxford, 1994.
6. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, 2nd, Ed. Butterworth-Heinemann,1997.

7. Russell S. Drago, Physical Methods for Chemists, 2nd Ed., Saunders College Publishing, 1992.

CHE 10803: Chemical Kinetics and Surface Chemistry (3 credits, 48 hrs.)

UNIT – I (10 hours)

Molecular reaction dynamics: Reactive encounters, Theories of reaction rates- Transition state theory, Comparative evaluation of collision and transition state theory, Thermodynamic treatment of reaction rates. Unimolecular reactions- Lindemann mechanism, Hinshelwood modification and RRK model.

Molecular beam methods, Stripping and rebound mechanism, Photsensitisation and quenching, Stern Volmer equation, Life time measurement

Fast Reactions- Relaxation methods- Perturbations, Flash photolysis and Pulse radiolysis

UNIT – II (8 hours)

Reactions in Solutions – Cage effect, Transition state theory for reactions in solutions, Diffusion controlled reactions, Effect of ionic strength, dielectric constant and Internal pressure, Primary and secondary salt effect

UNIT – III (8 hours)

Physical and chemical adsorption, adsorption isotherms- Langmuir (kinetic and statistical derivation), Freundlich and BET (derivation) isotherms, Determination of surface area using Langmuir and BET isotherms, Isosteric heat of adsorption. Thermodynamics of adsorption- Gibbs adsorption isotherm

UNIT – IV (12 hours)

Surface characterization techniques- Real condition analysis and need for Ultra High vacuum, Thermal desorption techniques (elementary introduction), Incident ion techniques- SIMS (Secondary Ion Mas Spectroscopy), SNMS (Secondary Neutral Mass spectroscopy), Microscopic techniques- SEM, TEM, AFM (elementary study). Surface and bulk scanning- XRD, XPS, UPS (basic principles)

UNIT – V (10 hours)

Catalysis and Inhibition, heterogeneous Catalysis – Transition state theory, General mechanism. General Mechanism of homogeneous catalysis- Arrhenius and vant Hoff intermediates, Acid base catalysis- specific and general acid catalysis, Unimolecular and bimolecular Surface reactions- Kinetics of adsorption- Langmuir Hinshelwood mechanism

and Rideal-Eley mechanism, Enzyme Catalysis- Michaelis-Menten Mechanism, Competitive and non competitive inhibition. Autocatalysis- Oscillatory reactions- Lotka-Volterra, Oregonator, Brussellator.

Catalysis by metals and semiconductors- electronic and geometric factors

Recommended Text Books:

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.

2. K. J. Laiddler, Chemical-Kinetics, McGraw Hill, New York.

3. M. R. Wright, An Introduction to Chemical Kinetics

4. Richard Masel, Chemical kinetics and Catalysis, Wiley Interscience

5. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York.

6. A. W. Adamson, The Physical Chemistry of Surfaces, 2nd Edn., Wiley. New York.

7. A. Somorjai, Chemistry of Surfaces, 3rd Edn. Wiley, New York.

8. D.P. Woodruff and T.A. Delchar, "Modern techniques of surface science", CambridgeUniversity press, 1990.

9. J.W. Niemantsverdriet, "Spectroscopy in Catalysis: an introduction", VCH, NY, 1995.

10. R. Pearce and W.R. Patterson, "Catalysis and chemical processes", Academic press, Leonard Hill, London, 1981.

11. Clark, "Theory of adsorption and catalysis", Academic Press, 1970.

12. J.M. Thomas & W.J. Thomas, "Introduction to principles of heterogeneous catalysis", Academic Press, New York, 1967.

13. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.

14. D.K Chakraborthy, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.

15. J.R. Anderson and M. Boudart (Eds), "Catalysis, Science and Technology", Vol

CHE 10804: Reagents and Organic Synthesis **(3 credits, 48 hrs.)**

UNIT – I **(10 hrs)**

Reagents: Reagents for oxidation and reduction: DDQ, PCC, activated DMSO oxidations, osmium tetroxide, selenium dioxide, singlet oxygen, peracids, hydrogen peroxide, periodic acid, lead tetraacetate., Woodward and Prevost hydroxylation, Sharpless and Jacobsen asymmetric epoxidation, Catalytic hydrogenations and dehydrogenation (heterogeneous and homogeneous), metal hydride reduction, Birch reduction, hydrazine and diimide reduction.

Synthetic applications of organometallic and organo-nonmetallic reagents: Reagents based on chromium, nickel, palladium, silicon, and boron, Gilman's reagent, phase transfer catalysts, Ziegler Natta catalyst, hydroboration reactions, synthetic applications of alkylboranes, C-H activation - Pd mediated coupling.

UNIT – II **(10 hrs)**

Chemistry of carbonyl compounds: Types of carbonyl compounds. enolization: thermodynamic and kinetic control, homoenolates. Darzen, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Baylis- Hilmann reaction, Michael additions and Robinson annulation. Reaction with phosphorous and sulfurylides, conversion of carboxylic acids to esters and amides.

UNIT – III **(10 hrs)**

Asymmetric Synthesis: Introduction to Asymmetric Synthesis, Principles, General strategies, Chiral Pool strategy, Chiral Auxiliaries-Diels Alder Reaction, Chiral Reagents – Binol Derivatives of $LiAlH_4$, Chiral Catalysts – CBS Catalyst. Stereospecific and Stereoselective Synthesis,

UNIT – IV **(10 hrs)**

Synthesis planning and analysis: Convergent, divergent and parallel synthesis, multicomponent reactions, concept of atom economy, Protection and activation of functional groups, functional group equivalents, reversal of reactivity (Umpolung), Chemistry of Nucleophilic Heterocyclic Carbenes (NHCs).

UNIT – V **(8 hrs)**

Retrosynthetic analysis: Introduction to retrosynthesis, disconnection approach-monofunctional, carboxylic acid and their derivatives, alkane, amine and bifunctional disconnections, synthesis of L-longifolene, Corey lactone, Djerassi - Prelog lactone, basic introduction to combinatorial chemistry.

Reccommended Text Books:

1. Smith, M. B. Organic Synthesis, 2nd Ed., McGraw-Hill, 2000.
2. Greene, T.W. and Wuts, P.G.M. Protecting Groups in Organic Synthesis, 2nd Ed., John Wiley, 1991.
3. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Ed., Wiley, 2013.
4. Bruice, P.Y. Organic Chemistry, 7th Ed., Prentice Hall Inc., 2013.
5. Morrison, R.T. Boyd, R.N. and Bhattacharjee, S.K. Organic Chemistry, 6th Ed., Pearson Education Inc., 2014.
6. Lowry, T H. and Richardson, K.S. Mechanism and Theory in Organic Chemistry, 3rd Ed., Benjamin-Cummings Publishing Company, 1997.
7. Carey, F. A. and Sundberg, R. J., Advanced Organic Chemistry (parts A and B), 5th Ed., Springer, 2008.
8. Pross, A. Theoretical and Physical Principles of Organic Chemistry, 1st Ed., Wiley, 1995.
9. Solomons, T.W.G. Fryhle, C.B., Snyder, S. A. Organic Chemistry, 12th Ed., Global, 2017.
10. Warren, S. Organic Synthesis: The Disconnection Approach, 2nd Ed., John Wiley, 2008.
11. House, H. O. Modern Synthetic Reactions, 2nd Ed., Benjamin-Cummings Publishing Co. Subs. of Addison Wesley Longman, 1972.
12. Carruthers, W. Some Modern Methods of Organic Synthesis, 4th Ed., Cambridge University Press, 2004.
13. Finar, I. L. Organic Chemistry Volumes 1 & 2, 6th Ed., Pearson Education Asia, 2004.

14. Flemming, I. Frontier orbitals and organic chemical reactions, Wiley-Blackwell, 1976.
15. Flemming, I. Molecular orbitals and organic chemical reactions, student edition, Wiley 2009.
16. Clayden, J. Green, N. Warren, S. and Wothers, P. Organic Chemistry, 2nd Ed., Oxford University Press, 2012.

CHE 10805: Organic Spectroscopy **(3 credits, 48 hrs.)**

UNIT – I **(8 hrs)**

Ultraviolet-Visible and Chirooptical Spectroscopy: Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules, estimation of λ_{max}

Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.

Chirooptical properties-ORD, CD, octant rule, axial haloketone rule, Cotton effect.

Problems based on the above topics.

UNIT – II **(8 hrs)**

Infrared Spectroscopy: Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

Problems on spectral interpretation with examples.

UNIT – III **(12 hrs)**

NMR Spectroscopy: Chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Higher order effects, examples of AB, AX, AA'BB' and ABX systems, simplification of higher order spectrum, application of NMR data for stereochemical assignments, ^{13}C NMR, selective decoupling, ^{1}H and ^{13}C chemical shifts to structure correlations. Application of DEPT technique in ^{13}C NMR spectroscopy, Illustration of practical applications of ^{1}H-^{1}H COSY, NOE difference spectroscopy (Stereochemistry determination), HMQC and HSQC techniques. Problems on spectral interpretation with examples.

UNIT – IV **(10 hrs)**

Mass Spectrometry: Molecular ion production methods (EI).

Soft ionization methods: FAB, CA, MALDI, PD, Field Desorption Electrospray Ionization. Fragmentation patterns, nitrogen and ring rules. McLafferty rearrangement and its applications.

HRMS, MS-MS, LC-MS, GC-MS. Problems on spectral interpretation.

UNIT – V **(10 hrs)**

Identification of structures of unknown organic compounds based on the data from MS, UV-Vis, IR, ^{1}H NMR and ^{13}C NMR spectroscopy. Interpretation of the given UV-Vis (including chiroptical data), IR and NMR spectra

Recommended Text Books:

1. Gunther, H. NMR Spectroscopy, 2nd Ed., John Wiley and Sons, 1995.
2. Pavia, D. L. Lampman, G. M. Kriz, G. S. Vyvyan, J. R.Spectroscopy, Cengage Learning, New Delhi, 2007.
3. Kemp, W. Organic Spectroscopy, 2nd Ed., ELBS-Macmillan, 1987.
4. Claridge, T.D.W. High Resolution NMR Techniques on Organic Chemistry, Pergamon, New York, 1999.
5. Macomber, R.S. A Complete Introduction to Modern NMR Spectroscopy, Wiley, 1997.
6. Nasipuri, D. Stereochemistry of Organic Compounds, Principles and Applications, 5th Ed., New Age International, New Delhi, 2014
7. Silverstein, R.M. Bassler, G.C. and Morril, T.C. Spectroscopic Identification of Organic Compounds, 5th Ed., Wiley, 1991.
8. Williams, D. H. Fleming, I. Spectroscopic Methods in Organic Chemistry, 5th Ed., McGraw-Hill, 1995.

CHE 10806: Chemistry Lab – Inorganic Mixture analysis

(2 credits, 64 hrs.)

Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li from a mixture of salts.

Inorganic preparations

Preparation of metalloporphrins

Recommended Text Books:

1. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.
2. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966
3. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.
4. Laboratory Manual, CHE 10806, Department of Applied Chemistry, CUSAT.

CHE 10807: Organic Chemistry Lab – (Multistep synthesis, purification and characterization)

(2 credits, 64 hrs.)

Preparation of organic compounds involving multistep synthesis

Purification and Characterization using spectroscopic techniques (IR, UV, NMR, GC-MS, emission spectra)

References:

1. Vogel's Textbook of Quantitative Chemical Analysis 6th edn, Pearsons Education Ltd.

2. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

3. F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

4. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

5. D. L. Pavia, G. M. Lampman, G. S. Kriz, Vyvyan, Introduction to Spectroscopy, 5th Ed., 2015.

6. Laboratory Manual, CHE 10807, Department of Applied Chemistry, CUSAT.

CHE 10808: Open Ended Lab **(2 credits, 64 hrs.)**

CHE 10809: Quantum Chemistry of Molecules and Macromolecules (Elective)

(2 credits, 32 hrs.)

UNIT - I **(8 hrs.)**

Chemical boning, Born Oppenheimer approximation, MO theory for the ground state and excited state of H_2^+, hydrogen molecule - MO treatment and calculation of energy, molecular term symbols, Molecular orbital method for diatomic molecules, Correlation diagram, Non-crossing rule. Valence bond method. H_2^+ and H_2 molecule, Comparison of VB and MO method, Bonding in simple molecules like water, BF_3, NH_3, CH_4, VSEPR theory, Pi bonding in simple molecules. HMO method for linear conjugated hydrocarbons, aromatic hydrocarbons, calculation of free valence charge density and reactivity.

UNIT – II **(6 hrs.)**

Molecular mechanics and force fields, various potential energy terms, parameterization, potential energy surface universal force fields - Fundamental molecular forces-the dynamic equation, ab initio methods - self consistent theory of molecules, Potential energy surfaces-Born – Oppenheimer approximation- geometry optimization- stationary points, local minima, global minima, saddle point and transition states, semiempirical methods and its basic principles. MINDO, AM1, PM3.

UNIT – III **(6 hrs.)**

Hartree Fock Self Consistent Field method, Slater's treatment of complex atoms, Slater orbitals. Restricted and unrestricted Hartree Fock- Pauli principle, Slater determinant and wave function., Roothan`s equations, Koopmans' theorem.

UNIT – IV **(6 hrs.)**

basis sets, Slater and Gaussian functions, classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets, Contracted Basis sets, pseudo potential.

UNIT – V **(6 hrs.)**

Hartree-Fock limit, electron correlation, Electron correlation – excited Slater determinants-configuration interaction. The UHF dissociation and the spin contamination problem. Many body perturbation theory- Moller-Plesset perturbation theory. Coupled Cluster theory. Introduction to Density Functional Theory (DFT) methods - Hohenberg-Kohntheorems, Kohn-Sham orbitals, exchange correlation functional, local densityapproximation, generalized gradient approximation and hybrid functionals. The Becke exchange correction. The Lee-Yang – Paar Correlation Potential, Conceptual DFT, Hybrid MM methods-mechanical embedding- IMOMM, IMOMO, ONIOM. Polarization embedding.

Recommended Text Books:

1. Atkins, P. W., Molecular Quantum Mechanics, 5th Ed., Oxford University Press, New York, 2010.
2. Mc Quarrie, D. A. Quantum Chemistry, 2nd Ed., University Science Books, 2007.
3. Prasad, R. K. Quantum Chemistry, 4th Ed., New Age Science, 2009.
4. Levine, I. N. Quantum Chemistry, 7th Ed., Pearson, 2013.
5. Szabo, A. and Ostlund, N. S. Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory, 2nd Ed., Dover, 1996.
6. Jensen, F. Introduction to Computational Chemistry, 3rd Ed., Wiley, New York, 2017.
7. Cramer, C. J. Essentials of computational Chemistry: Theories and models, 2nd Ed., John Wiley & Sons, 2004.
8. Parr, R.G. and Yang, W. Density Functional Theory of Atoms and Molecules, Oxford University Press, Oxford, 1989.
9. D. Young, Computational Chemistry: A Practical Guide to Real World Problems, Wiley, New York, 2001.
10. Haaland, A. Molecules and Models: The Molecular Structures of Main Group Element Compounds, Oxford University Press, Oxford, New York, 2008

CHE 10810: Adsorption and Catalysis (Elective) (2 credits, 32 hrs.)

Unit - I (8 hours)

Adsorption and catalysis – adsorption and reaction rate – strength of adsorption bond and catalysis – adsorption equilibrium and catalysis, kinetics of heterogeneous catalysis: diffusion steps neglected – unimolecular reactions – bimolecular reactions – Langmuir-Hinshelwood and Eley-Rideal mechanism, kinetics of heterogeneous catalysis: diffusion controlling – mechanism of diffusion – diffusion and reaction in pores – selectivity and diffusion, electronic factors in catalysis by metals, electronic factors in catalysis by semiconductors, geometric factors and catalysis.

Unit – II (6 hours)

Heterogeneous catalysis: Catalyst preparation methods – precipitation and coprecipitation – mechanism of nuclear formation and crystal growth, sol gel process–Dispersed metal catalysts; support materials; preparation and structure of supports; Synthesis of aluminosilicate zeolites and related silica-based materials, Mesoporous materials - ordered mesoporous materials – synthesis of silica and carbon molecular sieve materials. characterization of mesoporous molecular sieves

Unit – III (4 hours)

Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts

Unit – IV (10 hours)

Enzyme catalysis: catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis – specific catalytic groups contributing to catalysis – enzyme kinetics as an approach to understanding mechanism Characteristics of immobilized biocatalysts – activity as a function of temperature – stability as a function of temperature – temperature optimum in the long term process – the influence of pH value – influence of substrate concentration – influence of diffusion – other physical properties;

Unit – V **(6 hours)**

Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.

Recommended Text Books:

1. R. Pearce and W.R. Patterson, "Catalysis and chemical processes", Academic press, Leonard Hill, London, 1981.

2. Clark, "Theory of adsorption and catalysis", Academic Press, 1970.

3. J.M. Thomas & W.J. Thomas, "Introduction to principles of heterogeneous catalysis", Academic Press, New York, 1967.

4. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.

5. D.K Chakraborthy, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.

6. J.R. Anderson and M. Boudart (Eds), "Catalysis, Science and Technology", Vol 6, Springer-Verlag, Ber lin Heildberg, 1984.

8. R. Szostak, "Molecular sieves: principles of synthesis and identification", Van Nostrand, NY, 1989.

9. R. Hughes, "Deactivation of catalysts", Academic press, London, 1984.

10. A.L. Lehninger, "Principles of Biochemistry", Worth Publishers, USA, 1987.

CHE 10811: Crystallography (Elective) **(2 credits, 32 hrs.)**

Unit – I **(6 hours)**

Crystals, Obtaining crystals, Identification of crystal systems, cell parameters, asymmetric unit, unit cell, faces of crystal, Miller indices, Crystal symmetry, Space groups (symmorphic and non-symmorphic systems) , reciprocal lattice, Properties of a crystal

Unit – II **(6 hours)**

Significance of crystal structure determination by using X–rays as source, X-ray diffraction method, Bragg's law

Unit – III **(6 hours)**

Stages involved in crystal structure analysis by X-ray diffraction, experimental set up for single crystal X-ray analysis.

Unit – IV **(6 hours)**

Structure solution. Patterson and direct methods. Refinement techniques, R factor or discrepancy index

Unit – V **(8 hours)**

Crystal growth techniques – Solvothermal synthesis, Diffusion method, Slow evaporation method, Microwave Irradiation method, Sonochemical method, Mechanochemical method, Electrochemical method

Recommended Text Books:

1. R.S. Drago, "Physical Methods for Chemists", 2nd edition, Sauders College Publishing, 1992.

2. A Primer, J.P. Glusker and K.N. Trueblood, "Crystal Structure Analysis", 3rd edition, Oxford University Press Inc., New York, 2010.

3. C Giacavazzo (Ed.), H.L. Monaco, G. Artioli, D. Viterbo, M. Milanesio, G. Ferraris, G. Gilli, P. Gilli, G. Zanotti, M. Catti, (Ed.), “Fundamentals of crystallography”, 3rd edition, Oxford Science Publications, Oxford University Press, 2011.

4. J. D. Dunitz, “X-ray analysis and the structure of organic molecules”, 2nd edition Wiley-VCH, 1996.

5. G.H. Stout and L.H. Jensen, “X-ray structure determination: A practical guide”, 2nd edition, Wiley Interscience Publications, 1989.

CHE 10812: Bioanalytical Chemistry (Elective) **(2 credits, 32 hrs.)**

Unit – I **(8 hours)**

Biomolecules- amino acid, protein, nucleic acid –structures, physical and chemical properties, features and characteristics of major biomolecules, structure-function relationship, significance.

Analyses and quantification of biomolecules- method to detect and quantify biomolecules.

Unit – II **(6 hours)**

Principle of centrifugation, concept of RCF, features and component of major types of centrifuge, preparative, differential and density gradient centrifugation, analytical ultra-centrifugation, centrifugation methods for bio analysis. Determination of molecular weight.

Unit – III **(6 hours)**

Electrophoretic techniques- Principles of electrophoretic separation. Types of electrophoresis including paper, cellulose, acetate/nitrate and gel. Electroporation, Pulse field gel electrophoresis- applications in life and health science.

Unit – IV **(6 hours)**

Radio immune assay (RIA) - principle and applications. Enzyme linked immune sorbent assay (ELISA) principle and applications. Biosensors-applications

Unit – V **(6 hours)**

Transmission and scanning, freeze fracture techniques, specific staining of biological materials.

Recommended Text Books:

1) Understanding bio analytical chemistry-principle and applications-Victor A. Gault and Neville. H. Mcclenaghan.John Wiley and Sons, Ltd Publications 2009

2) Bio analytical Chemistry- Andreas Manz.: Nicole Pamme. Dimitri Iossifidis.2004

3) Bio analytical chemistry- Suson R. Mikkelsen, Eduaro Corton- John Wiley and Sons, Ltd Publications

4) Practical Biochemistry-Principles and techniques: -Keith Wilson and John Walker 5th edition, cambridge University press (2000)

CHE 10901: Organometallic and Bioinorganic Chemistry (3 credits, 48 hrs.)

UNIT – I (8 hrs.)

Compounds with transition metal to carbon bonds: classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: Metal nitrosyls, cyanides and isocyanides. structure, bonding, spectra, preparation and reactions; transition metal organometallics.

UNIT – II (10 hrs.)

Transition metal clusters. Parallels with nonmetal chemistry isolobal analogy. Metal alkyls, carbenesand carbines Nonaromatic alkene and alkyne complexes allyl and pentadienyl complexes metallocenes structure of cyclopentadienyl compounds arene complexes, complexes of cycloheptatriene,cyclooctatetraene and cyclobutadiene complexes metal clusters Application of Wade-Mingos-Lauher rules in predicting the structure of organometallic clusters and comparison with mno rules in predicting the stability of macropolyhedral boranes

UNIT – III (10 hrs.)

Main group organometallics – preparation and use as synthetic reagents, substitution reactions, oxidative addition, reductive elimination and insertion reactions, Grignard reagents, organolithium compounds, organoberyllium and magnesium compounds, organoboranes, organometallic compounds of aluminium, silicon and tin, preparation and properties of transition metal – alkyl and aryl compounds

UNIT – IV (10 hrs.)

Homogeneous catalysis using organometallic compounds: Reactions of organometallic complexes Ligand cone angle oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack of coordinated ligands olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation.

UNIT – V (10 hrs.)

Metal ions in biological systems: Chlorophylls, photosynthesis, heme proteins, hemoglobin, myoglobin, hemerythrin, hemocyanin, cytochromes and vitamin B12; Iron-sulphur proteins: rubredoxin, ferredoxin and model systems. Copper enzymes, superoxide dismutase, cytochrome oxidase and ceruloplasmin; Coenzymes; Molybdenum enzyme: xanthine oxidase; Zinc enzymes: carbonic anhydrase, carboxy peptidase and interchangeability of zinc and cobalt in enzymes; Vitamin B12 and B12 coenzymes; Iron storage, transport, biomineralization and siderophores, ferritin and transferrins. Applied bioinorganic chemistry, anti-cancer agents–cisplatin, radiopharmaceuticals (Tc), diagnostic (Gd in MRI) and therapeutic agents. Boron neutron capture therapy of cancer.

Recommended Text Books:

1. Purcell, K.F & Kotz, J.C. Inorganic Chemistry, 2nd Ed., W.B. Saunders Co, 1991.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L. Inorganic Chemistry, Principle and structure and reactivity, 4th Ed., Harper Collins College Publishers, New York, 1993.
3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry 2nd Ed., University Science Books, 1994.
4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. 6th Ed., Wiley-Interscience, 1999.
5. Basolo, F, and Pearson, R.C., Mechanisms of Inorganic Chemistry, 2nd Ed., John Wiley & Sons, NY, 1967.
6. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, 2nd., Ed. Butterworth-Heinemann,1997.
7. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
8. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint, Pearson Education, 2005.
9. Douglas, B. E.; McDaniel, D.H. and Alexander, J.J. Concepts and Models in Inorganic Chemistry 3rd Ed., John Wiley and Sons, NY, 1994.
10. Powell, P. Principles of Organometallic Chemistry, 2nd Ed., Springer, 1991.
11. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
12. Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals. 6th Ed., New York, NY: John Wiley, 2014.

13. W. L. Jolly, Modern Inorganic Chemistry, McGraw-Hill International, 2nd Edition, New York, 1991.
14. Gupta, B. D. and Elias, A. J. Basic Organometallic Chemistry, 2nd Ed., University Press, 2013.
15. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
16. Kaim, N. and Schwederski, B. Bioinorganic Chemistry: Inorganic Elements in the Chenistry of Life, 2nd Ed., John Wiley, 2013.

CHE 10902: Advanced Solid State and Electrochemistry (3 credits, 48 hrs.)

UNIT – I (9 hours)

Activity and Activity coefficient of electrolytes, Ionic strength, Debye Huckel theory of strong electrolytes, Debye Huckel limiting law equation, Application of Debye Huckel theory to conductance bahaviour, Relaxation and electrophoretic effect, Debye-Huckel-Onsager equation and its derivation- Application of Debye Huckel equation for the determination of thermodynamic equilibrium constants, Calculation of effect of ionic strength on the reaction rates in solutions. Debye Falkenhagen effect. Wein effect.

UNIT – II (9 hours)

Equilibrium Electrochemistry-EMF Phenomena, Cell Potential and its measurement, reference electrodes, Electrochemical series, Calculation of thermodynamic properties and activities, Cells without liquid junction potential, Liquid junction potential and its determination, Determination of solubility. Conductometric, Potentiometric and pH titrations, Redox indicators and redox titrations.

UNIT – III (10 hours)

Dynamic Electrochemistry- Electrical double layer, Various models of electrical double layer, Electrode polarization. Electrolytic polarization, Dissolution and deposition potential, Overpotential and its theories, Butler Volmer equation, Tafel equation. Tafel plot and its significance, Overvoltage- hydrogen overvoltage and oxygen overvoltage, Theories of hydrogen overvoltage.

Corrosion and methods for prevention. Porbaux diagram and Evans diagrams.

Storage cells- Lithium ion battery.

Fuel Cell. Theory and working of fuel cell. H_2- O_2 fuel cell, Methanol fuel cell, Solid oxide fuel cells, alkaline and polymer electrolyte fuel cells.

Introduction to electrocatalysis.

UNIT – IV (10 hours)

Review of Crystal symmetry and symmetry elements and symmetry operations, crystal systems, Bravais lattices and crystal classes, Crystallographic point groups - Schönflies & Hermann–Mauguin

notations, Stereographic projections of the 27 axial point groups, translational symmetry elements & symmetry operations - screw axes and glide planes, Introduction to space groups. Bragg's law and applications, lattice planes and miller indices, *d*-spacing formulae, crystal densities and unit cell contents,

Imperfections in solids - point, line and plane defects, non-stoichiometry

UNIT – V **(10 hours)**

Electronic structure of solids – free electron theory, band theory & Zone theory, density of states, band structure, direct and indirect band gaps, Brillouin zones; Electrical properties - electrical conductivity, Hall effect, dielectric properties, piezo electricity, ferro-electricity and ionic conductivity; Superconductivity- Meissner effect, brief discussion of Cooper theory of superconductivity; Low temperature and high temperature superconductivity, Optical properties - photo conductivity, luminescence, colour centers, lasers, refraction & birefringence; Magnetic properties - diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism & ferrimagnetism; Thermal properties - thermal conductivity & specific heat

Solid state reactions: Brief introduction.

Recommended Text Books:

1. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Edn., Wiley, New York, 1998
2. 2. R. Crow, Principles and Applications of Electrochemistry, Paper back edn, 4th edn, 1994.
3. S.Glasstone, An Introduction to Electrochemistry, Paperback edn., 2007
4. L.V.Azaroff, Introduction to Solids, Mc Graw Hill, 1960.
5. A. R. West, Solid State Chemistry, Wiley Student (Indian) Ed., (2014)
6. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967.
7. Lesley Smart and Elaine Moore, Solid State Chemistry, Chapman and Hall, 1995.
8. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.
9. C. N. R. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry. 2nd edn, Cambridge Uty Press, 1997.

CHE 10903: Chemistry of Natural Products **(3 credits, 48 hrs.)**

UNIT – I **(10 hrs)**

Introduction to heterocyclic compounds - 3, 4, 5 & 6 membered rings containing one or two heteroatoms - Nomenclature synthesis and reactions.

UNIT – II **(10 hrs)**

Fused ring compounds: indole, quinoline, isoquinoline, coumarin, flavone, anthocyanins, purine and pyrimidine bases present in nucleosides. Structure of porphyrins, hydroporphyrins, phthalocyanins, synthesis of porphyrin and phthalocyanins.

UNIT – III **(10 hrs)**

Terpenoids: classification and biosynthesis of terpenoids; structure elucidation and synthesis of abietic acid;

UNIT – IV **(10 hrs)**

Steroids: Classification and biosynthesis, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone.

UNIT – V **(8 hrs)**

Alkaloids - classification, isolation, structure elucidation based on degradative reactions (quinine and atropine only). Biosynthesis of quinine and papaverine.

Recommended Text Books:

1. Smith, M.B. Organic Synthesis, 2nd Ed., McGraw-Hill, 2000.
2. Finar, I. L. Organic Chemistry Volumes 1 & 2, 6th Ed., Pearson Education Asia, 2004.
3. Krishnaswamy, N. R. Chemistry of Natural Products; A Unified Approach, 2nd Ed., Universities Press, 2010.
4. Simmonds, R. J. Chemistry of Biomolecules: An Introduction, RSC, 1992.
5. Joule, J. A. Mills, K. Heterocyclic Chemistry, 5th Ed., Wiley, 1998.

CHE 10904: Biological Chemistry **(3 credits, 48 hrs.)**

UNIT – I **(8 hrs)**

Cell Structure and Function: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells.

Introduction of biomolecules: Examples of biomolecules and building blocks of biopolymers. Types of reactions occurring in cells, structure of ice and liquid water, hydrogen bonding and hydrophobic interactions, buffers and the Henderson-Hasselbalch equation.

UNIT – II **(8 hrs)**

Carbohydrates: Monosaccharides, oligosaccharides and polysaccharides, Synthesis of Vitamin C from glucose, biosynthesis of shikimic acid, inositol and its derivatives. Carbohydrates of glycolipids and glycoproteins, role of sugars in biological recognition, blood group substances.

Introduction to metabolism: Overview of metabolism, catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation.

UNIT – III **(8 hrs)**

Lipids and membranes: Common classes of lipids - glycerolipids, phospholipids, sphingolipids and glycolipids. Self-association of lipids - formation of micelles, reverse micelles and membranes, gel and liquid-crystalline phases. Lipid phase polymorphism - bilayer, hexagonal and cubic phases. Liposomes and their properties and applications. Biological membranes and the fluid mosaic model, current models of biological membranes, membrane proteins and their functions, membrane asymmetry.

UNIT – IV **(12 hrs)**

Amino acids, peptides and proteins: Synthesis of aminoacids - Strecker and azalactone synthesis, enantioselective synthesis of aminoacids, reactions of aminoacids. Primary structure of proteins, end group determination, amino acid analysis and the Edman degradation (protein sequencing), Ramachandran plot and the secondary structure of proteins

α-helix, β-pleated sheet, β-bend and collagen triple helix. Tertiary structure and structural motifs - protein folding and domain structure of proteins. Oligomeric proteins. Purification and characterization of proteins, functions of proteins.

Enzymes and catalysis: Substrate specificity of enzymes, requirement of coenzymes, regulation of enzyme activity and allosteric effect, enzyme nomenclature, enzyme kinetics and the MichaelisMenten equation, function of chymotrypsin, NAD, thiamine, pyridoxal. Various types of enzyme inhibition. Application of enzymes in chemical synthesis, enzyme models and their applications.

UNIT – V **(12 hrs)**

Nucleotides and nucleic acids: Ribonucleotides and deoxyribonucleotides, RNA and DNA. Base pairing, double helical structure of DNA and forces stabilizing nucleic acid structure. Methods used in nucleic acid separation and characterization, nucleic acid sequencing.

Transcription and translation: Messenger RNA, RNA polymerase and protein synthesis. Control of transcription and protein - DNA interactions. The genetic code, tRNA structure and codonanticodon interactions. Ribosomes and their structure. Gene cloning and site-directed mutagenesis.

Recommended Text Books

1. Voet, D. and Voet, J. G. Biochemistry, 4th Ed., John Wiley, 2010.
2. Nelson, D.L. and Cox, M.M. Lehninger Principles of Biochemistry, 5th Ed., W. H. Freeman and CBS Publishers, 2008.
3. Berg, J. M. Tymoczko, J. L. and Stryer, L. Biochemistry, 5th Ed., W. H. Freeman, 2002.

CHE 10905: Computational Chemistry Laboratory (2 credits, 64 hrs.)

Computational calculations using programming package - Building of molecular structure, molecular geometry optimization, conformational analysis, thermodynamic and spectroscopic properties, molecular orbital analysis electron density and electrostatic potential map.

Recommended Text Book:

1. J. Foresman and A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
2. Laboratory Manual, CHE 10905, Department of Applied Chemistry, CUSAT.

CHE 10906: Chemistry Laboratory - Instrumentational (2 credits, 64 hrs.)

POTENTIOMETRY

Measurement of electrode potentials

Potentiometric Titrations

REFRACTOMETRY

Variation of refractive index with composition

Determination of unknown composition

CONDUCTOMETRY

Cell constant

Solubility of a sparingly soluble salt

Conductometric Titrations:

CV STUDIES

SPECTROPHOTOMETRY

UV, IR, Flame photometry, AAS

Recommended Text Books:

1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan, 2014.
2. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. Laboratory Manual, CHE 10906, Department of Applied Chemistry, CUSAT.

CHE 10907: Open Ended Laboratory **(2 credits, 64 hrs.)**

CHE 10908: Computational Chemistry (Elective) (2 credits, 32 hrs.)

UNIT – I (8 hrs.)

Scope of computational chemistry, Introduction to molecular mechanics; comparison of popular force fields; performance of molecular mechanics, Molecular dynamics, the fundamental concepts of quantum mechanics - Schrödinger equation, Born-Oppenheimer approximation, potential energy surfaces, local and global minima, transition states, variational method, LCAO, Hartree-Fock theory, restricted HF calculations; open shell systems, ROHF and UHF calculations, Roothan–Hall equations, Koopmans theorem, HF limit and electron correlation,

UNIT – II (6 hrs.)

Basis sets, basis set approximation, Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, classification of basis sets – minimal, double zeta, triple zeta, correlation-consistent sets, core-valence sets, general contractions, EMSL basis set exchange, Semi empirical methods, post Hartree-Fock Method, Configuration interaction, Many-body perturbation theory, Coupled-cluster theory, Nondynamical correlation and multiconfigurational self-consistent-field (MCSCF) theory, Density Functional Theory, Comparing the performance of electronic structure theories, Hybrid QM/MM

UNIT – III (6 hrs.)

Input of molecular structure, Z-matrix construction, single point energy calculations, geometry optimizations, Electronic Energy, Vibrational frequency analysis, symmetry analysis, zero-point vibrational energies (ZPVE's), distinguishing minima from transition states, Intrinsic reaction coordinate (IRC) analysis, transition barrier and activation energy, conformational energetics, reaction energetics, enthalpy of formation, bond dissociation energy, ionization energy, isomerization energy and barrier, potential energy surface, reaction mechanism, enthalpy, entropy and free energy changes for reactions, isodesmic reactions.

UNIT – IV (6 hrs.)

Analysis of gaussian output files, dipole moment, multipole moments, polarizability, hyperpolarizability, and molecular electrostatic potential, partial atomic charges, thermodynamic properties, atomic spin, ionization potentials, electron affinities, infrared spectra and NMR spectra, use of graphics programs like Chemcraft, Molden in analyzing Gaussian output data, identification and visualization of normal modes of vibration, calculation and interpretation molecular orbitals

UNIT – V **(6 hrs.)**

Determination of molecular properties using molecular mechanics, ab initio, semi empirical and DFT methods. Wave function analysis- population analysis. Geometry, Total energy, Dipole moment, vibrational frequency, Chemical Shifts. Determination of orbital energy gap – electronic spectral transitions. Application to polymers- periodic boundary condition. Determination of polarizability and hyperpolarizability of organic molecules and polymers. Interaction with solvents and solvent effects- Onsager model. Solvatochromism.

Recommended Text Books:

1. Cramer, C. J. Essentials of computational Chemistry: Theories and models, 2nd Ed., John Wiley & Sons, 2004.
2. Jensen, F. Introduction to Computational Chemistry, 3rd Ed., Wiley, New York, 2017.
3. Leach, A. R. Molecular Modelling Principles and Applications, 2nd Ed., Pearson Education Limited, 2001
4. Szabo, A. and Ostlund, N. S. Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory, 2nd Ed., Dover, 1996.
5. Mc Quarrie, D. A. Quantum Chemistry, 2nd Ed., University Science Books, 2007.
6. Levine, I. N. Quantum Chemistry, 7th Ed., Pearson, 2013.
7. Cotton, F. A. Chemical Applications of Group Theory, 3rd Ed., Wiley, New York, 1990.
8. Wilson, E. B., Decius, J. C. and Cross, P. C. Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover, New York, 1980.

CHE 10909: Green Chemistry (Elective) **(2 credits, 32 hrs.)**

UNIT – I **(3hrs.)**

Green Chemistry and industry, waste minimization, E factor and atom economy, Reduction of- material use, energy, risk and hazards. Sustainable use of- chemical feedstocks, water, energy. LCA methodology, Renewables as Chemical Feedstocks and Biocatalysis, Process Intensification for Green Chemistry.

UNIT – II **(8hrs.)**

Catalysis in green chemistry – Homogenous catalysis, Heterogeneous catalysis, metal catalysts, metal oxide catalyst, metal complexes, Solid Acid Catalysts - Concepts and applications, Zeolite, Heteropolyacid, Ion-exchange resins as solid acid catalysts, Kvaerner Process, Nafion /silica nanocomposites, Haldor–Topsoe alkylation process to high-octane fuels. Micelle-templated Silica as Catalysts in Green Chemistry - Synthesis of micelle templated materials, Catalytic Applications - Oxidation catalysis, Base catalysis, Enantioselective catalysis.

UNIT – III **(5hrs.)**

Phase-transfer Catalysis(PTC) - Classical PTC Reactions, Nucleophilic aliphatic and aromatic Substitutions, Phase-transfer catalysis elimination and isomerisation reactions, Base-promoted alkylation and arylation, Inverse PTC, Phase-transfer Catalysis in Polymerisation, Applications of PTC in Analytical Chemistry. Biocatalysis - antibody catalysts, Enzyme Catalysts, Biomimetic catalysts, Chemical Production by Biocatalysis, Bulk chemicals, Pharmaceuticals, Flavour and fragrance compounds, Carbohydrates, Polymers, Biocatalysis in supercritical CO_2, Biocatalysis in waste treatment.

UNIT – IV **(8hrs.)**

Specific green technologies - hydrogen peroxide in waste minimization, waste minimization in pharmaceutical process development, supercritical carbon dioxide as an environmentally benign reaction medium for chemical synthesis, reduction of volatile organic compound emission during spray painting. Extraction of natural product with super-heated water, Synthesis at organic – water interface, Envirocats, applications of microwaves for environmentally benign organic chemistry, Sonochemistry – Concept, application in chemical synthesis.

UNIT – V **(8hrs.)**

Photochemistry - Photons as Clean Reagents, Reduced usage of reagents, Lower reaction temperatures, Control of selectivity, Photochemical reactions for industry, General Problems with Photochemical Processes, Specialized photochemical reactors and process technology, Photochemical reactors, Light sources, Artificial Photosynthesis for small molecule conversions. Green Nanoscience - Photocatalysis by Nanostructured TiO_2-based Semiconductors, Formation of Nanoparticles Assisted by Ionic Liquids, Nanoencapsulation for Process Intensification, Nanophase Inorganic Materials, Nanomaterials from Biobased Amphiphiles.

Recommended Text Books:

1. Paul T. Anastas and John C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, 1998.
2. J. Clark, D. Mcquarrie, *Hand Book of green Chemistry and technology*, Blackwell science, 2002.
3. Mike Lancaster, *Green Chemistry: An Introductory Text*, RSC, 2007.
4. P. T. Anastas, T. C. Williamsons, *Green Chemistry – Designing Chemistry for the Environment*, ACS, 1994.
5. V. K. Ahluwalia, M. Kidwai, *New Trends in Green Chemistry*, 2nd edition, Anamaya Publishers, 2006.
6. V. K. Ahluwalia, *Green Chemistry*, Narosa Publishing House, 2011.
7. Alvise Perosa, Maurizio Selva, *Handbook of Green Chemistry- Volume 8- Green Nanoscience*, Wiley-VCH, 2012.

CHE 10910: Electroanalytical Techniques (Elective) **(2 credits, 32 hrs.)**

Unit – I **(8 hours)**

Ionics: Electrochemistry of solutions, Ion-solvent interactions, ion-ion interactions, ionic migration and diffusion.Electrodics: Faradaic and non Faradaic processes, Concept of surface excess, Electrical double layer- Theories of Double-Layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern Model, Adsorption of ions and neutral compounds, Electrocaplillary and differential capacitance measurements; Influence of double layer on charge transfer processes.

Unit – II **(4hours)**

Working and Reference electrodes: polarizable and non-polarizable systems, Butler Volmer equations, Tafel equations

Unit – III **(10 hours)**

IR drop and polarization, Mass transport, Linear diffusion, Fick's laws and diffusion coefficient

Voltammetry-Principle and instrumentation, two electrode and three electrode system, Excitation signals- Linear sweep, Cyclic, Differential pulse and Square wave, Different types of current-Diffusion, migration and convection, Residual current, Half wave potential, Role of supporting electrolyte, Randles Sevcik equation, Use of microelectrodes in voltammetry, Cyclic voltammetry in reversible, quasi-reversible and irreversible systems, Study of reaction mechanisms, Surface modification in charge transfer and interfacial activity, Impedance Spectroscopy

Unit – IV **(4 hours)**

Modification of electrodes using nanomaterials, conducting polymers, voltammetric sensors and electrocatalysis, Controlled Potential Techniques

Stripping voltammetry- Anodic and cathodic, Polarography-Dropping Mercury electrode– advantages and disadvantages, Ilkovic equation, Amperometry and Chronoamperometry, Chronopotentiometry

Unit – V **(8 hours)**

Controlled potential and controlled current techniques

Principle, Instrumentation and Applications of Electrogravimetry without potential control and Controlled potential electrogravimetry

Principle, Instrumentation and Applications of Controlled potential coulometry, Coulometric titrations

Recommended Text Books:

1. Allen J. Bard and Larry R. Faulkner, Electrochemical Methods: Fundamentals and Applications, 2nd edition 2001, John Wiley & Sons
2. D. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, 6th Edition, Brooks/Cole Cengage Learning, Belmont, CA, 2007
3. D. A. Skoog, D.M. West, F. J. Holler and S. R. Crouch, Fundamentals of Analytical Chemistry, 8th Edition, Brooks/Cole Cengage Learning, Belmont, CA
4. Bockris, J. O. M.; Reddy, A. K. N. Modern Electrochemistry, Volume 2A, Fundamentals of Electrodics; Kluwer Academic/Plenum Publishers: New York, 1998.
5. Monk, P. M. S. Fundamentals of Eletroanalytical Chemistry; Wiley: Chichester, 2001.
6. Willard, H. H.; Merritt, L. L.; Dean, J. A.; Settle, F. A. Instrumental Methods of Analysis; 6th Edn, D. Van Nostrand Co: New York, 1981.

CHE 10911: Advanced Photochemistry (Elective) **(2 credits, 32 hrs.)**

UNIT – I **(6 hrs.)**

Energy Transfer-Theories of Energy Transfer – Photosensitization of Organic and Inorganic Molecules – Singlet Oxygen – Methods of singlet oxygen generation and Detection – Chemistry of Singlet Oxygen – Photodynamic Therapy of Cancer

UNIT – II **(6 hrs.)**

Photoinduced Electron Transfer – Theory of Electron transfer – Circumventing Back Electron transfer – Photoinduced Electron transfer reactions of Organic and Inorganic Molecules – Photosynthesis –

UNIT – III **(6 hrs.)**

Photochemistry and Photophysics of Semiconductors – Semiconductor Photocatalysis and applications. Atmospheric photochemistry.

UNIT – IV **(8 hrs.)**

Photochemistry and Advanced Materials - Artificial Solar Energy Harvesting – Photochemical Splitting of Water – Dye sensitized solar cells - Grätzel Cell - Bulk heterojunction devices for solar energy harvesting - Organic light emitting devices.- Photoresists – Photolithography – Photochromism – Photonic Materials and Lasers

UNIT – V **(6 hrs.)**

Photochemistry in Practice – Radiometry and Actinometry – Priciples of Radiometry and radiometers – Actinometry – Quantum Yields – Light Sources – Optical Materials and Filters – Photochemical Reactors

Recommended Text Books:

1. Nicholas J. Turro, V. Ramamurthy, Juan C. Scaiano, Modern Molecular Photochemistry of organic molecues, University Science Books, 2010.
2. Carol E. Wayne, Photochemistry (Oxford Chemistry Primers), 1st Ed., Oxford University Press, 1996.
3. Joseph R. Lakowicz, Principles of Fluorescene Spectroscopy, 3rd Ed., Plenum Press, 2010.

4. Andre M. Braun, Photochemical Technology, Marie-Therese Maurette, Esther Oliveros, John Wiley & Sons, 1991.

5. Marye Anne Fox, M. Chanon, Photoinduced Electron Transfer by Part A, B. C and D, Elsevier Science Publishing Company, 1988.

6. J.,Ed. Mattay, Photoinduced Electron Transfer 1-5 (Topics in Current Chemistry), 1st Ed., Springer, 1990-1993.

7. G. J. Kavarnos, Fundamentals of Photoinduced Electron Transfer, 1st Ed., Wiley-VCH, 1993.

8. Molecular and Supramolecular Photochemistry, Volume 10, Semiconductor Photochemistry and Photophysics , Editors, V. Ramamurthy and K. Schanze, Marcel Dekker: New York, 2003.

9. Photochemistry in Organized and Confined Media, Editors, V. Ramamurthy, VCH Publishers, New York, 1991.

CHE 10912: Microbial Technology (Elective) **(2 credits, 32 hrs.)**

UNIT – I **(6 hrs.)**

Industrial microorganisms: differentiation between prokaryotes and eukaryotes; General characteristic, structures, nutrition, growth, reproduction and economic importance of bacteria, Economic importance of fungi and acinomycets

Prevention and control of microorganisms- Control by physical and chemical agents-

UNIT – II **(8 hrs.)**

Fermentation techniques: Screening procedures; preservation and maintenance of industrial microorganisms; batch, fed batch and continuous fermentation. Fermentor.

Down stream processing- Introduction, separation- filtration, centrifugation, flocculation and flotation; disintegration of cells-mechanical and nonmechanical methods; extraction. Concentration methods-evaporation, membrane filtration, ion exchange. Purification-chromatography, drying and crystallization.

UNIT – III **(6 hrs.)**

Manufacture of Beer, Production of alcohol by fermentation.

Manufacture of diary products- Butter, Cheese. Fermented milk beverages- kefir, kumiss. Yoghurt. Microbial production of antibiotic- Penicillin, streptomycin.

UNIT – IV **(6 hrs.)**

Microbial production of Organic acids and Amino- Citric and acetic acid; glutamic acid, lysine. Microbial production of vitamins- vitamin B12 and Riboflavin

Microbial transformation of steroid and sterol.

UNIT – V **(6 hrs.)**

Production and purification of microbial enzymes- protease, amylases, lipases and their industrial application. Enzyme immobilization- various methods of immobilization and application of immobilized enzymes.

Recommended Text Books:

1. P F. Stanbury, A Y Whitaker and S J Hall, “Principle of Fermentation Technology Elsiever, 2003, online published 2007

2. Pelzar, Reid and Chan, “Microbiology” McGraw Hills Inc., New York, 1979

3. Casida L.E, Industrial Microbiology, 1984

4. Peppler and Pearlman, Microbial Technology, Academic press, 1979

5. John B'uock and Bjorn Kristansen, Basic Biotechnology, Academic Press, 1987

CHE 10913: Advanced Solid-State Chemistry (Elective) (2 credits, 32 hrs.)

UNIT – I (6 hrs.)

Band theory of solids- energy bands, conductors and non-conductors, intrinsic semiconductors, extrinsic semiconductors, Hall effect.

UNIT – II (8 hrs.)

Stoichiometric Defects: Equilibrium concentration of point defects in crystals - Schottky defects, Frenkel defects; The photographic process - light sensitive crystals, mechanism of latent imageformation, lithium iodide battery.Non-Stoichiometric Defects: Origin of non-stoichiometry, consequences of non-stoichiometry; Equilibria in non-stoichiometric solids, Color centers: F-centre, electron and hole centre; colour centre and information storage.

UNIT – III (5 hrs.)

Electrical properties; conductivity in pure metals; superconductivity; basics, discovery and high Tc superconductors magnetic properties; ferromagnetic and antiferromagnetic materials

UNIT – IV (5 hrs.)

Optical properties; photoconductivity, photovoltaic effect, applications, luminescence. Electrical properties: dielectric properties, piezo-electricity, Ferro electricity. Lasers and their applications in chemistry.

UNIT – V (8 hrs.)

Preparative methods: Solid state reaction, chemical precursor method, co-Precipitation, sol-gel, metathesis, self-propagating high temperature synthesis, ion exchange reactions, intercalation/deintercalation reactions; hydrothermal and template synthesis; , preparation of thin films - electrochemical methods, chemical vapour deposition; Crystal growth - Bridgman & Stokbarger methods, zone melting.

Characterization of Solids: Crystal growing; Data collection, data reduction, refinement and structure solution of some compounds

Recommended Text Books:

1. R. West. Solid State Chemistry and its Applications, John Wiley, 1987.
2. N. B. Hannay, Solid State Chemistry, Prentice Hall of India, 1979.

3. R. J. D. Tiley. Defect Crystal Chemistry and its Applications, Chapman and Hall, NewYork, 1987.
4. L.V. Azaroff, Introduction to Solids, Mc.Graw Hill, New York, 1960.
5. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967.
6. Lesley Smart and Elaine Moore, Solid State Chemistry, Chapman and Hall, 1995.
7. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.

CHE 10914: Polymer Technology (Elective) **(2 credits, 32 hrs.)**

UNIT – I **(6 hrs.)**

Classification of elastomers. Manufacture, properties, processing, compounding, vulcanisation and applications of SBR, polybutadiene and polyisoprene rubber. Comparison of synthetic polyisoprene with NR. Manufacture, properties, processing, compounding, vulcanisation and applications of EVA, Polyacrylate rubbers, Polysulphide rubbers and Polyurethanes.

UNIT – II **(5 hrs.)**

Manufacture, properties, processing, compounding, vulcanisation and applications of EPDM, Butyl rubber, Nitrile rubber, Neoprene rubber, Hypalon rubber, Silicone rubber and Fluorocarbon rubber.

UNIT – III **(5 hrs.)**

Brief history of plastics - Advantages and disadvantages - thermoplastics and thermosets. Manufacture of monomers, polymerization and structure of poly vinyl chloride, characterization of commercial polymers, compounding ingredients, PVC formulations. Some simple moulding techniques- Injection moulding, Compression moulding, and Blow moulding.

UNIT – IV **(8 hrs.)**

Manufacture of phenolic resins, preparation of phenol formaldehyde moulding powders, applications of PF resin. Urea formaldehyde resin and applications of UF resin. Adhesives-adhesive bonding-advantages-adhesive classification - basic terminology-theories of adhesion-wettability -performance of adhesives -shear, peel and cleavage properties-factors affecting adhesive performance. Structural adhesive -types -epoxy, urethane, acrylic, phenolic and high temperature and PVC plastisol types, advantages and disadvantages.

UNIT – V **(8 hrs.)**

Mechanical properties of plastics and rubber – tension, compression, shear, flexural, tear strength,dynamic stress- strain, hardness, impact strength, resilience, abrasion resistance, creep and stress relaxation, compression set, dynamic fatigue, ageing properties etc. Thermal properties– specific heat, thermal conductivity, thermal expansion, heat deflection

temperature etc. Electrical properties– resistivity, dielectric strength, dielectric constant etc. Optical properties – transparency, refractive index, haze, gloss etc.

Recommended Text Books:

1. Rubber Technology Handbook, Werner Hofman, Hanser Publications, 1989.
2. Rubber Technology and Manufacture, C M Blow, Butterworths, London, 1971.
3. Plastics Materials, J. A. Brydson, Butterworth Heinmann, 1999.
4. Industrial Polymers, Ulrich, Hanser Pub. Munich, N.Y, 1982.
5. Adhesives in manufacturing, Gerald L. Schnberger, Marcel Dekker Inc., New York, 1983.
6. W. C. Wake, Adhesion and the formulation of adhesives, Applied Science Publishers, London ,1976.
7. R. P. Brown, Plastic test methods, Harlond, Longman Scientific, 1992.
8. Vishu Shah, Handbook of Plastic Testing Technology, John Wiley & Sons, New York,1998.
9. R. P. Brown, Physical Testing of Rubbers, Chapman hall, London, 1996.
10. J. F. Rabek, Experimental methods in Polymer Chemistry, John Wiley & Sons, New York, 1980.
11. F. Majewska, H. Zowalletal, Handbook of analysis of synthetic polymers and plastics, Ellis Horwood Limited Publisher, England, 1977.
12. C. A. Harper, Handbook of Plastics Elastomers & Composites, 2nd Ed., McGraw Hill Inc. New York 1992.
13. Rubber Technology, Maurice Morton ,VanNostrand Reinhold , Handbook,1987.
14. V. R. Gowariker, N. V. Viswanathan and Sreedhar, Polymer Science, Wiley Eastern Limited, New Delhi, 1986.

CHE 10915: Chemistry of Carbohydrates (Elective) (2 credits, 32 hrs.)

UNIT – I (6 hrs.)

Definition and classification of sugars, nomenclature, aldoses and ketoses, configuation of (+)- glucose: the Fischer proof, ring structures and conformation, mutarotation, anomericity, naturally occurring monosaccharides, oligosaccharides and polysaccharides, three-dimensional structure of macromolecular carbohydrates. Introduction to Inositol and its derivatives and their commercial applications.

UNIT – II (6 hrs.)

Methods for isolation, purification and structural analysis, complete and partial hydrolysis, methylation analysis, Smith degradation, color tests and methods for estimation of carbohydrates.

UNIT – III (8 hrs.)

Chemical ractions of carbohydrates, oxidation, reduction, formation of derivatives, glycosides, ethers, esters and cyclic acetals, modern chemical transformations, methods for the formation and cleavage of O-glycosidic bond, use of protecting groups, Formation of acetals between diols, Regioselective opening and deprotection of acetals, Esterifications, Ester deprotections, Alkylations, Silylations, Nitrogen protections. Conversion of glucose to ascorbic acid.

UNIT – IV (6 hrs.)

Chemical and enzymatic synthesis of oligosaccharides, carbohydrates as chiral synthons for natural products synthesis. Nucleophilic Displacement on Carbohydrate Rings.

UNIT – V (6 hrs.)

Carbohydrate biopolymers, animal glycoproteins, blood-group substances, plant and algal glycoproteins, proteoglycans and glycosaminoglycans, glycolipids, glycoconjugates, carbohydrate components of nucleic acids and antibiotics.

Recommended Text Books:

1. J.F. Kennedy and C.A. White, Bioactive Carbohydrates, Ellis Horwood, New York, 1983.
2. R.W. Binkley, Moden Carbohydrate Chemistry, Marcell and Dekker, New York.,1988
3. J.F. Kennedy (Ed.) Carbohydrate Chemistry, Oxford University Press, Oxford, 1988.

4. E.A. Davidson, Carbohydrate Chemistry, Holt, Rinehart & Winston Inc., Mew York, 1967.
5. A.F.Bochkov and G.E. Zaikov, Chemistry of the O-Glycosidic Bond Formation and Cleavage, Pergamon, Oxford, 1979.
6. S.Hanessian, Total Synthesis of Natural Products: The Chiron Approach, Pergamon, Oxford. 1983.
7. Essentials of Carbohydrate Chemistry and Biochemistry", 3rd ed, by Thisbe K. Lindhorst.Wiley VCH 2007.
8. Carbohydrate Chemistry (Oxford Chemistry Primers) B. G. Davis and A. J. Fairbanks, Oxford University Press 2002.

CHE 10916: Medicinal Chemistry (Elective) **(2 credits, 32 hrs.)**

UNIT – I **(6 hrs.)**

Principles of Drug discovery: Introduction to drug discovery. drug discovery without lead – serendipity – Pencillins, Cisplatin, librium (chlordiazepoxide), aspertame as examples. Selection of disease and drug target.Bioassay and Lead discovery.Drugs from natural sources and development.

Case studies of modification of morphine and atropine. Drug metabolism studies: Phase I and Phase II metabolism. Clinical observations: Phase I, Phase II, Phase III, Phase IV trials (Introductory treatment only).

Principles of drug design; agonist, antagonist drugs, Structure pruning technique in drug design (eg. morphine pharmacophore). Development of ranitidine and captopril from lead molecules.Introduction to combinatorial synthesis.Drug resistance and mutation.

UNIT – II **(6 hrs.)**

SAR Studies: Introduction to structure-activity relationship (SAR) studies – (i) Binding role of hydroxyl group, amino group, aromatic ring, double bond, ketones and amides, (ii) Variation of substituents – alkyl substituents, aromatic substituents, extension of structure, chain extension / contraction, ring expansion / contraction, ring variation, ring fusion, Isosteres. (iii) Simplification of the structure, rigidification, conformational blockers. X-ray crystallographic studies. Case studies of oxaminquine (schistosomiasis), sulpha drugs (antibacterial), benzodiazepines (hypnotic).

UNIT – III **(6 hrs.)**

QSAR Studies: Introduction to Quantitative Structure Activity Relationship (QSAR) studies. QSAR parameters – substituent constants – linear and non – linear relationships between ρ and biological activity. Electronic parameters, steric parameters, effect of electronic and steric parameters on lipophilicity. Methods used in QSAR studies – (i) Linear free energy relationship (LFER). Application of Hammett equation. (i) Hansch analysis – significance of slopes and intercepts in Hansch analysis, (ii) Craig's plot, (iii) Topliss scheme, (iv) Free Wilson model – advantages and disadvantages, (v) Clustet significant analysis (vi) Minimal topological difference method.

UNIT – IV **(8 hrs.)**

Selected Drugs–I (Chiral drugs: Synthesis/production and mode of action): Introduction to chiral drugs. Eotomer, distomer, eudesmic ratio, three point contact model – Feiffers rule. Synthesis of [S]-Ibuprofen and [S]-Naproxen (non-steroid anti-inflammatory drugs); Digoxin Propranolol, Atenolol and Metoprplol (Cardiovascular drugs); Ramipril and Quinapril (ACE inhibitors); [2S,3S]-Diltiazem (Calcium antagonist) Paroxetine (Serotonin uptake inhibitor); Indanavirsulfate (crixivan, HIV-I protease inhibitor); Lamivudine (3TC, HIV-reverse transcriptase inhibitor), Fexofenadine (H-blocker), thalidomide (immunomodulator), oral contraceptives.

UNIT – V **(6 hrs.)**

Selected Drugs-II: Synthesis/production and mode of action: Penicillins, cephalosporins, valinomycin, gramicidin, tetracyclins, chloramphenicol, erythromycin, ciprofloxacin, isoniazid, prontosil (Antibacterial agents). Ivermectin (antiparasitic) Aspirin (analgesic), Aciclovir, azidothymidine, saquinavir, ritonavir, oseltamivir (Antiviral agents).Genistein, camptothecin, podophyllotoxin, calicheamicin, tamoxifen, paclitaxel (Anticancer agents). Salbutamol, ephedrine, Phenobarbital, prozac (CNS Drugs).Salvarsan (Antisyphilitic). Lovastatin (cholesterol lowering), cyclosporine (immunosuppressant).Viagra (vascodialator).Methadone (narcotic).

Recommended Text Books:

1. An Introduction of Medicinal Chemistry, by G. L. Patrick, 3rd Edition, 2006, Oxford International Edition, Oxford University Press.

2. Organic Chemistry of Drug Design and Action, R. B. Silverman, 2nd Edition, 2004, Academic Press, Sandiego.

3. Medicinal Chemistry: An Introduction, G. Thomas, John Wiley and Sons, 2nd Edition, 2007,John Wiley and Sons.

4. Abraham, D. J. (Ed). Berger's Medicinal Chemistry, 6th Edition, Vol 1-6, John Wiley and Sons, New York, 2003.