Definitions

CC	Core Course is a common course in the subject and is compulsory.
DSEC	Discipline Specific Elective Course is a specialized paper within the subject. In lieu of DSEC, student can opt for alternative papers from MOOCs SAYAM platform in 1st and 2nd Semester up to 3 papers (12 credits).
GEC	Generic Elective Course is a course to be offered to the allied/unrelated subjects.
SEC	Skill Enhancement Course is a vocational aspect of the subject.
RM	Research Methodology and proposal writing.

(All papers have 4 credit weightage)

FIRST SEMESTER		
Paper Code	**Paper**	**Minimum credit reqd**
CHE-CC-500	Physical Chemistry I (Quantum Chemistry & Spectroscopy)	4
CHE-CC-501	Organic Chemistry I (Laboratory Course)	4
CHE-DSEC-502	Inorganic Chemistry I (Theory)/MOOCs	4
CHE-DSEC-503	Physical Chemistry II (Theory)/MOOCs	4
CHE-GEC-504	Environmental Chemistry	4
	Total	**20**
SECOND SEMESTER		
CHE-CC-505	Physical Chemistry III (Theory)	4
CHE-CC-506	Inorganic Chemistry II (Laboratory Course)	4
CHE-DSEC-507	Organic Chemistry II (Theory)/MOOCs	4
CHE-DSEC-508	Interdisciplinary Chemistry/MOOCs	4
CHE-RM-509	Research Methodology & Proposal writing	4
CHE-SEC-510	Analytical Methods in Chemistry	4
	Total	**24**
THIRD SEMESTER		
CHE-CC-600	Organic Chemistry III (Theory)	4
CHE-CC-601	Physical Chemistry IV (Practical)	4
CHE-CC-602	Inorganic Chemistry III (Theory)	4
CHE-DSEC-603	Industrial Techniques in Inorganic Chemistry	4
CHE-DSEC-604	Organic Chemistry IV (Research Tools for Organic Chemistry)/MOOCs	4
CHE-DSEC-605	Physical Chemistry V (Research Tools in Physical Chemistry)/MOOCs	4
	Total	**24**
FOURTH SEMESTER		
CHE-DSEC-606	Research Project/Dissertation	20
	Total	**20**

First Semester **CHE-CC-500** **Credits: 4**

PHYSICAL CHEMISTRY-I

Unit 1: ***Principles of Quantum Mechanics, Application to Model Systems and Approximate Methods***
Review of the basic principles of quantum mechanics: Postulates, operators and related theorems, Schrödinger equation, normalization and orthogonalization of wave function. Expectation values, Quantum mechanical operators, Hamiltonian operator, Hermitian operators, angular momentum operator. Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential and tunnelling, hydrogen atom. Approximation methods: Variation and time-independent perturbation methods (up to 2^{nd} order) and simple applications.

Unit 2: ***Chemical Bonding***
Many-electron wave functions and anti-symmetry principle; Born-Oppenheimer approximation; valence bond (VB) and molecular orbital (MO) approaches for diatomic molecules, LCAO-MO treatment of hydrogen molecule ion, hydrogen molecule; bonding and anti-bonding orbital; Comparison of LCAO-MO and VB treatments of H_2 and their limitations; excited states of H_2 - singlet and triplet; term symbols; hybridization; Huckel MO treatment for conjugated π-electron systems.

Unit 3: ***Rotational and Vibrational and Electronic Spectroscopy***
Introduction: Interaction of light with matter, mechanism of absorption and emission of radiation.

(A) Rotational and Vibrational Spectroscopy
Degrees of freedom of molecules; rigid rotor model; rotational spectra of diatomics and polyatomics; effect of isotopic substitution and nonrigidity; selection rules and intensity distribution. Vibrational spectra of diatomics; effect of anharmonicity; Morse potential; Vibration-rotational spectra of diatomics; P, Q, R branches, normal modes of vibration, overtones, hot bands. Raman spectroscopy: Origin; rotational and vibrational Raman spectra of diatomics.

(B) Electronic Spectroscopy
Electronic spectroscopy: Electronic spectra of diatomic molecules, Franck-Condon principle, Vibronic transitions, Spectra of organic compounds, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition.

(C) Photochemistry
Types of photophysical pathways, Radiationless transitions, Fluorescence emission, Triplet state and phosphorescence emission.

Unit 4: ***Magnetic Resonance Spectroscopy***

(A) Nuclear Magnetic Resonance: Nuclear spin and nuclear spin states in magnetic field, resonance phenomenon, relaxation processes, NMR line shapes and saturation, shielding and de-shielding of magnetic nuclei, chemical shift, spin-spin interactions, spectra of a two-spin system (A_2, AB and AX cases), ^{13}C, ^{19}F, and ^{31}P NMR spectroscopy.

(B) Electron Spin Resonance: Basic principles, factors affecting g values, hyperfine coupling, spin densities and McConnell relationship. Zero field splitting.

Text Books

1. D. A. McQuarrie, *Quantum Chemistry*, Viva books, 2020.
2. D. A. McQuarrie and J. D. Simon, *Physical Chemistry*, Viva books, 2020.
3. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 5th Ed., Tata McGraw-Hill, New Delhi, 2015.

Reference Books

1. P. W. Atkins and R. Friedman. *Molecular Quantum Mechanics*, 4^{th} Ed., Oxford University Press, 2005.
2. R. McWeeny. *Coulson's Valence*, ELBS, 1979.
3. J. D. Graybeat. *Molecular Spectroscopy*, McGraw-Hill Int. Ed. 1988.

First Semester **CHE-CC-501** **Credits: 4**

Organic Chemistry I
(LABORATORY COURSE)

PART A

1. Purification Techniques of organic compounds and their spectroscopic identifications.
   a) Purification of binary mixtures by Thin Layer Chromatography (TLC) and Column chromatography (CC).
   b) Purification of tertiary mixtures of amino acids by Paper Chromatography.

2. Extraction of Natural Products: Any one of the following – solasodine, caffeine, nicotine, piperine, rosine, carotenoids, curcumin, citral.

3. Organic Preparations: At least eight preparations (involving two or more than two steps) involving the following representative reactions-
   a) Esterification and saponification
   b) Oxidation (peracid, chromic acid, Mn(Vll)
   c) Hydride reduction or hydrogenation
   d) Nucleophilic substitution
   e) Cycloaddition reaction
   f) Grignard reaction
   g) Condensation reaction
   h) Preparation of dyes
   i) Aromatic electrophilic substitution
   j) Heterocyclic synthesis

4. Qualitative Analysis of Binary Mixtures (only two)

PART B

Principle, instrumentation, handling, precautionary measures, experiment, data collection and analysis of the following instruments:

a) IR
b) HPLC and GC
c) Microwave

Text Books

1. R. K. Bansal. *Laboratory Manual of Organic Chemistry* (3rd edn.), Wiley-Eastern (1994).
2. R. G. Brewster & W.E. Mcwedn. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).
3. A. I. Vogel. *Practical Organic Chemistry* (3rd edn.), Longman Group Ltd. (1973).

Reference Books

1. A. O. Fitton & R. K. Smallery. *Practical Heterocyclic Chemistry* Academic Press (1968)
2. R. L. Shriner & R. C. Fuson. *Systematic Identification of Organic Compounds* (5th edn.), John Wiley & Sons (1964).

First Semester **CHE-DSEC-502** **Credits: 4**

Inorganic Chemistry - I

Unit 1: ***Symmetry and Group Theory:*** Symmetry elements and operations; equivalent symmetry elements and equivalent atoms; Identification of symmetry point groups with examples from inorganic compounds; groups of very high symmetry; molecular dissymmetry and optical activity; systematic procedure for symmetry classification of molecules and illustrative examples; molecular symmetry for compounds having co-ordination numbers 2 to 9; Brief review of matrix representation of group, reducible and irreducible representations; Application to molecular vibration.

Unit 2:

(a) ***Metal-Ligand Equilibria in Solution***: Stepwise and overall formation constants; trends in stepwise formation constants; determination of binary formation constant by spectrophotometry; factors affecting stability of metal complexes and chelate effect.

(b) Reaction Mechanism of Transition Metal Complexes: Discussion on general reactivity of metal complexes, Labile and inert complexes; mechanisms of ligand-replacement reactions; ligand displacement reactions in square planar and octahedral complexes; *trans* effect; electron transfer reactions: outer sphere and inner sphere, atom transfer; isomerisation and racemisation of tris-chelate complexes; stereochemical nonrigidity and fluxional molecules.

Unit 3: ***Magnetochemistry:*** Brief review of different types of magnetic substance and magnetic behaviour, measurement of magnetic susceptibility, Magnetic moment for single and multi-electron system, L-S and j-j coupling, Ground State Term symbols for metal ions; R-S coupling and Lande intervals, Spin-orbit coupling, Thermal energy and magnetic property: temperature-independent paramagnetism, application of crystal field to explain the magnetic properties of coordination compounds: Magnetic moment of first row transition metal ions, spin crossover, quenching of orbital magnetic moment, Magnetic properties of Lanthanides and Actinides, Antiferromagnetic interactions in inorganic compounds: direct interaction and super exchange mechanism.

Unit 4: ***Electronic Structure of Transition Metal Complexes:*** Electronic absorption spectra and colour of octahedral and tetrahedral complexes, selection rules, Orgel diagrams, Tanabe- Sugano diagrams, calculation of Dq, B and ß values, band intensities and band widths, spectra of high-spin octahedral and tetrahedral complexes of d^1 to d^9 systems, Spectrochemical series; Adjusted crystal field theory, Nephelauxetic series, Molecular orbital theory of complexes, MO diagrams for octahedral and tetrahedral complexes and charge-transfer spectra, optical properties of Lanthanides and Actinides.

Text Books

1. J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi *Principles of Structure and Reactivity* (1st impression), Pearson Education (2006).
2. F. A. Cotton *Chemical Applications of Group Theory*, (3rd edn.), John Wiley & Sons (1999).
3. R. L. Dutta and A. Syamal, *Elements of Magnetochemistry* (2nd Edn), EWP (2010)
4. J. D. Lee, *Concise Inorganic Chemistry* (5th Edn) John Wiley & Sons (1996).

Reference Books

1. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong. *Shriver and Atkins Inorganic Chemistry*, Oxford University Press (2006).
2. N. N. Greenwood & A. Earnshaw. *Chemistry of the Elements*, Pergamon Press (1984).
3. F. Basolo & R. G. Pearson, *Mechanism of Inorganic Reactions*, Wiley Eastern (1967).
4. S. F. A. Kettle, *Physical Inorganic Chemistry*, Spectrum (1996).

First Semester **CHE-DSEC-503** **Credits: 4**

PHYSICAL CHEMISTRY - II

Unit 1: *Electrochemistry*-I

Ion–ion Interaction: Debye-Huckel theory of ion-ion interaction; Poison equation, Linearized Poisson–Boltzmann equation; ionic cloud and chemical potential change; activity coefficients and mean ionic activity coefficients; expression of mean ionic activity coefficients in terms of ionic strength.

Ion-solvent interaction: free energy change due to ion-solvent interactions; Born model; enthalpy and entropy of ion-solvent interactions.

Unit 2: *Electrochemistry*-II

Electrodics: processes at electrodes, electrical double layer; Helmholtz-Perrin model; Gouy-Chapman diffuse charge model and Stern model. The basic electrodic equation: Butler–Volmer equation; overpotential; polarizable and nonpolarizable interfaces, Corrosion.

Unit 3: *Solid State Chemistry*

Review of the basic concepts: Bragg's law, Miller indices, Elements of symmetry (plane, axis and centre of symmetry). X-ray diffraction: powder method, principle and applications.

Crystal Defects: Point defects, Stoichiometric and non-stoichiometric defects, Kroger-Vink notation for crystal defects.

Metals, insulators and semiconductors; intrinsic and extrinsic semiconductors, p-n junction.

Solid Solutions: Substitutional, interstitial and subtractional solid solutions & distortions.

Unit 4: *Surface Chemistry*

Surface tension and surface free energy; Pressure across an interface: Laplace equation, Kelvin equation; Wetting: Young-Dupre equation; Adsorption in liquid systems: Gibbs adsorption isotherm.

Surfactants, classification of surfactants, hydrophobic interaction, aggregation/micellization of surfactants, critical micelle concentration (cmc), factors affecting the cmc, thermodynamics of micellization: phase separation and mass action models. Sols of surface-active reagents, electrical properties of colloidal systems, size determination of colloidal particles.

Text Books

1. J. O'M Bockris and A. K. N. Reddy. *Modern Electrochemistry*, Plenum, New York, 2007.
2. D. A. McQuarrie and J.D. Simon –*Physical Chemistry*, VIVA Students Ed., 2003.
3. A. R. West. *Solid State Chemistry and its Applications*, John Wiley,1998.
4. Y. Moroi. *Micelles: Theoretical and Applied Aspects*, Plenum, 1992 (Softcover reprint of the original 1st ed. 1992 edition: 20 November 2013).

First Semester **CHE-GEC-504** **Credits: 4**

ENVIRONMENTAL CHEMISTRY

Unit 1: Water pollution and Remediation

(a) Environmental cycles: Global water, carbon, nitrogen phosphorus cycles

(b) Water Quality parameters: Physico-Chemical Water Quality Indicators (Electrical conductivity, dissolved oxygen, BOD and COD); Effect of inorganic and organometallic compounds; heavy metals and metalloids; and radionuclides on the water quality; nonaqueous-phase liquids (NAPLs) and pesticides as organic water pollutants.

Unit 2: (a) Wastewater Treatment and Related Technologies: Primary, secondary and tertiary treatment process of municipal sewage and water; disinfection by chlorination, ozonation and ultraviolet radiation; Use and disposal of biosolids; Point-of-entry (POE) and point-of use (POU) technologies for water treatment; Advanced Oxidation Processes (AOPs) for wastewater treatment.

(b) Environmental and Health Impacts of Uranium and Coal Mines.

Unit 3: The Atmosphere and Associated Processes

The layers of the atmosphere; atmospheric radiation and photochemical reactions - Stratospheric ozone formation and the role of VOCs and NOx, Stratospheric ozone destruction and the role of halogen compounds; Biosphere-Atmosphere interactions (biogenic and anthropogenic emissions);

Unit 4: Air Pollution and its Removal Process: Photochemical smog; greenhouse effect; Peroxyacetyl nitrate (PAN) formation and NOx transport; Aldehydes in the atmosphere; Heterogeneous atmospheric reactions; Atmospheric deposition processes for removal of pollutants.

Text Books

1. G. Hanrahan, Key Concepts in Environmental Chemistry, Elsevier Inc. (2012), ISBN: 978-0-12-374993-2.
2. N. Gupta, R. S. Khoiyangbam, and N. Jain, Introduction to Environmental Sciences, Ch. Environmental Chemistry, pp. 15-49, Teri Press (2015).
3. R. Mahapatra, S. S. Jeevan, S. Das, (Eds); Environment Reader for Universities, Centre for Science and Environment, New Delhi (2017).

Second Semester **CHE-CC-505** **Credits: 4**

PHYSICAL CHEMISTRY - III

Unit 1: ***Reaction Kinetics-I***
Determination of rate laws: Integral, isolation, half-life and differential methods; comparison of different techniques. Kinetic equations for complex reactions: Chain, parallel, opposing and consecutive reactions; Enzyme catalysis. Enzyme Inhibition reactions, Michaelis-Menten mechanism.

Unit 2: ***Reaction Kinetics-II***
Theory of reaction rates; Temperature effect on reaction rates; Rate constant for simple bimolecular reactions; Collision theory; Activated complex theory, Lindemann, Hinshelwood and the RRKM theories for unimolecular reactions, Reactions in solutions: Diffusion controlled & activation-controlled reactions; Thermodynamic formulation of rate constant: effect of pressure & ionic strength. Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed unimolecular & bimolecular reactions; Concept of potential energy surface for a reaction.

Unit 3: ***Statistical Thermodynamics***
(A) Phase space, ensembles, different types of ensembles, ensemble averaging, concept of distribution, distribution law (Boltzmann statistics), partition function, relation between molecular and molar partition functions, thermodynamic parameters in terms of partition function, equilibrium constant in terms of partition function. Translational partition function, rotational partition function for linear and non-linear molecules; vibrational partition function, electronic partition function, reference state of zero energy for evaluating partition function.

(B) Application of statistical thermodynamics: equipartition theorem, heat capacity behaviour of crystals. Introduction to quantum statistics: Distribution law for fermions (Fermi-Dirac statistics) and for bosons (Bose-Einstein statistics), and its applications.

Unit 4: ***Non-Equilibrium Thermodynamics***
Entropy of irreversible processes – Clausius inequality; entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy flow; Entropy production in open systems; Rate of entropy production – generalized forces and fluxes; Phenomenological equations, Onsager reciprocity relation; Electrokinetic phenomena; Stationary non-equilibrium states -states of minimum entropy production.

Text Books

1. K. J. Laidler, *Chemical Kinetics* (4th Edn.), Pearson Eductions, 2007.
2. D. A. McQuarrie and J.D. Simon –*Physical Chemistry*, VIVA Students Ed., 2003.
3. P. W. Atkins & J. de Paula. Physical Chemistry (8th edn.), OUP, 2006.
4. D. A. McQuarrie. Statistical Mechanics, Viva Books Pvt. Ltd., New Delhi, 2003.
5. C. Kalidas and M. V. Sanganarayana. *Non-Equilibrium Thermodynamics – Principles and Applications*, Macmillan India, 2002.

Reference Book

1. P. L. Houston, Chemical Kinetics & *Reaction Dynamics*, Dover, NY, 2006.
2. K Huang, *Statistical Mechanics*, OUP, 2006.
3. I. Prigogine. *Introduction to Thermodynamics of Irreversible Processes*, Interscience, 1960.

Second Semester **CHE-CC-506** **Credits: 4**

INORGANIC CHEMISTRY - II (Laboratory Course)

1. Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometiric methods of constituents in three component mixtures and alloys.

2. Preparation and Characterization of the following compounds (at least 5 preparations are to be completed by turn):

    (a) Tris(acetylacetonato) iron(III)
    (b) Tris(acetylacetonato)manganese(III)
    (c) Reinecke salt
    (d) Tris(oxalate) manganese(III)
    (e) Tetrapyridinesilver(II)peroxidisulphate
    (f) Bis(*N*,*N*-diethyldithiocarbamato)nitrosyliron(I)
    (g) Optical isomers of tris(ethylenediamine)cobalt(III)chloride
    (h) Linkage isomers of nitro and nitritopentamminecobalt(III) chloride
    (i) Hydridochlorocarbonyl tris(triphenylphosphine)ruthenium(II)
    (j) $[(p\text{-(cymene)}RuCl_2]_2$

3. Synthesis and characterization of metal Schiff base complex.
   Characterization includes microanalysis, and conductance measurements and FTIR, UV-Visible, NMR spectroscopy and cyclic voltammetry studies.

Text Books

1. J. Mendham, R. C. Danney, J. D. Barnes & M. Thomas. *Vogel's Textbook of Quanti-tative Chemical Analysis*, Peterson Education (2000).
2. G. Marr & B. W. Rockett. *Practical Inorganic Chemistry*, Van Nostrand (1972).
3. G. Pass & H. Sutcliffe. *Practical Inorganic Chemistry* (2nd edn.), Chapman & Hill (1974)

Reference Books

1. J. Basset, R. C. Denney, G.H. Jeffery & J. Mendham. *Vogel's Text Book of Quantitative Analysis* (4th edn.), English Language Book Society (1978).
2. H. H. Willard, L. L. Merrit & J. A. Dean. *Instrumental Methods of Analysis* (4th edn.), East-West Press (1974).
3. G. W. Parshall (Ed. in Chief). *Inorganic Synthesis*, Vol. 15, McGraw Hill, p. 48 (1974).

Second Semester **CHE-DSEC-507** **Credits: 4**

ORGANIC CHEMISTRY - II

Unit 1: (a) Stereochemistry: Axial and planar chirality, helicity; topicity and prostereoisomerism; Racemic modification and optical purity; Conformational analysis of acyclic, cyclic, heterocyclic and steroidal systems; Effects of conformation on reactivity.

(b) Reactive Intermediates I: Concept, generation, stereochemical aspects, and important name reactions of carbenes, nitrenes, and arynes.

Unit 2: (a) Pericyclic Reactions: Main features of pericyclic reactions; Woodward-Hoffman rules, correlation diagram and FMO approaches; Electrocyclic reactions – conrotatory and disrotatory motions for 4n and 4n+2 systems; Cycloadditions – antarafacial and suprafacial additions, [2+2] and [4+2] reactions (hν and Δ), 1,3-dipolar cycloadditions and chelotropic reactions; Sigmatropic [i,j] shifts of C-H and C-C bonds; Sommelet-Hauser, Claisen, thio-Claisen, Cope and aza-Cope rearrangements.

(b) Photochemistry: Photochemistry of alkenes and carbonyl compounds; photochemistry of aromatic compounds; concept and applications of photochemical isomerisation, addition and substitution reactions.

Unit 3: (a) Aromaticity and Reaction mechanisms: Concept and application of aromaticity, Aromaticity in benzenoid and non-benzenoid compounds, *n*-annulenes, heteroannulenes, fullerenes, cryptates; Mechanism, stereochemical aspects and application of addition, elimination and substitution reaction. Concept of E, Z geometry of enolates, kinetic vs thermodynamic control of enolates, stereoselective enolate reactions – alkylation and aldol condensation (Zimmerman models).

(b) Reactive Intermediates II: Concept, generation, stereochemical aspects, and important name reactions of free radicals; Barton reaction and Hoffmann-Loefller-Freytag reaction.

Unit 4: Reactions and Reagents: Stereochemistry and application of catalytic hydrogenation, hydride reduction, hydroboration, dissolving metal reductions, and carbonyl reduction with hydrazine derivatives; Oxidation of alcohol with PCC, PDC, Collin's reagent, Swern oxidation, IBX, Dess-Martin periodinane, MnO_2, Ag_2CO_3 on celite; oxidation of alkene with peracids, metal/alkyl hydroperoxides, Sharpless asymmetric epoxidation and asymmetric dihydroxylation, dioxiranes, I_2/Ag^+ ; periodates, LTA, SeO_2; Photo-Fries rearrangement of ethers and anilides; di-π-methane rearrangement; Photooxygenation - Singlet molecular oxygen reactions.

Reference Books:

[1] D. Nasipuri, Stereochemistry of Organic Compounds, 2nd Edn, New Age International (1994).
[2] P. S. Kalsi. Stereochemistry, Conformation and Mechanism (7th edn.), New Age (2008).
[3] C. Depuy & O. L. Chapman. Molecular Reactions and Photochemistry, Prentice-Hall of India (1975).
[4] March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure (6th edn.), Wiley Student Edition, John Wiley & Sons Asia Pte. Ltd. (2006).
[5] F. A. Carey & R. J. Sundberg. Advanced Organic Chemistry Part B, Plenum Press, 5th edition (2008).
[6] M. B Smith. Organic Synthesis (2nd end.), McGraw-Hill, Inc. (2001).
[7] T. L. Gilchrist & C. W. Rees, Carbenes, Nitrenes and Arynes, Nelson, London (Reprinted 2008).

Second Semester **CHE-DSEC-508** **Credits: 4**

INTERDISCIPLINARY CHEMISTRY

Unit 1: ***Inorganic photochemistry I*****:** Introduction to inorganic photochemistry, photophysical and photochemical process, characteristics of the electronically excited states of inorganic compounds, ligand field states, charge transfer states; Photochemical processes: Selection rules, Jablonski diagram, Fluorescence and phosphorescence, delayed fluorescence, Photochromism, Photosensitization, Quantum yield; Photochemical reactions: substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes; organometallic photochemistry;

Unit 2: ***Inorganic photochemistry II*****:** Luminescent d^6 and d^{10} complexes; Molecular recognition, Sensing, Bioimaging, Supramolecular chemistry, Photochemical splitting of water, Dye sensitized solar cells, Photoredox catalysis.

Unit 3: (a) ***Polymer chemistry:*** Concept of polymerization, classification, mechanism of polymerization, characterization, co-polymerization, ionic polymerization, thermoplastic, thermosetting polymers, natural and artificial rubber, vulcanization, plasticizer and elastomers.

(b) ***Supramolecules:*** Concept, nature of supramolecular interactions, host-guest chemistry, crown ethers, cryptands, cyclodextrins, calixarenes, molecular recognition: cations, anions, neutral molecules binding hosts, molecular devices.

Unit 4: (a) ***Co-Enzyme****:* Structure & function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid and vitamin B_{12} in biological processes.

(b) ***Nucleic acids:*** Primary, secondary and tertiary structure of DNA; DNA replication and heredity; Structure and function of *m*RNA, *t*RNA and *r*RNA. Role of ATP in biological processes.

Suggested Books

1) D. M. Roundhill. *Photochemistry and Photophysics of Metal Complexes*, Plenum Press (1990). 5.
2) J. E. Huheey, E. A. Keiter & R. L. Keiter, *Inorganic Chemistry* (4^{th} edn) Prentice Hall (1997)
3) N. J. Turro, V. Ramamurthy, J. C. Scaiano, *Principles of Molecular Photochemistry: An introduction*, University Science Books (2009).
4) David Nelson, Lehninger Principles of Biochemistry 8th Edition, W.H. Freeman
5) M. S. Bhatnagar. *A textbook of polymer chemistry*, Vol (I-III): S. Chand and Company (2004).
6) J. W. Steed and J. L. Atwood. *Supramolecular Chemistry*: Willy Reprinted (2002).

Second Semester **CHE-RM-509** **Credits: 4**

Research Methodology and Proposal Writing

Unit 1: Research methodology: Definitions, Purpose of Research, Types of research, Research approaches, Research Methods, Stages of the research process, Background reading & information gathering: Literature survey, Hypothesis: Identification of Research Problem; Ethical issues in research, Data collection, Data recording and reproducibility, Importance of documentation.

Unit 2: Research ethics and Publication: Presentation of research findings: Elements of research publications; Seminar presentation; Patent; Paper writing; Journal impact factor, h-index; review process.

Unit 3: Laboratory safety: General health and safety concerns; What to do after splash/cut, Chemical hazards, commonly used hazardous laboratory chemicals (azide, perchlorate, nBuLi, acid chlorides, bromine, cyanide, mercury, etc), Personal protective equipment, Environmental safety issues: Fume hood safety, Safety data sheet, Waste handling, Disposal of chemical and plastic-waste; precautionary measure for the maintenance of laboratory equipment.

Unit 4: *Statistical Methods and Computer Applications in Chemistry*: Errors, precision and accuracy; Average Mean Deviation, Standard Deviation, Variance, Chi-square Test. Applications of Curve Fitting, Straight Line Fitting, Interpolation in solving chemical problems. Applications of commonly used Computer Softwares, such as Chemdraw, Chemoffice, Mercury, Origin, Excel, etc.

Reference Books

1. National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). *On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition.* National Academies Press.
2. K. Prathapan, *Research Methodology for Scientific Research*, Dreamtech Press (2019)
3. R. Ridley, *Handbook of Good Laboratory Practices*, 2nd Edition, WHO (2009).
4. Ramesh Kumari, *Computers and their Applications to Chemistry*, 2nd Ed., Narosa Publishing House, 2007.
5. K. Atkinson, *Elementary Numerical Analysis*, 2nd Ed., John Willy and Sons, 2003.
6. R. Ridley, *Handbook of Good Laboratory Practices*, 2nd Edition, WHO (2009).

Second Semester **CHE-SEC-510** **Credits: 4**

ANALYTICAL METHODS IN CHEMISTRY

1. Hands on training on evaluation of analytical data to determine Relative error, Indeterminate error, source of error, The Normal law of Error; Statistical evaluation of data: Mean, Median, Mode, Deviation, Average/Mean deviation, Standard deviation, Variance, Probable deviation, Precision of the mean: average, standard and probable deviation of the mean; Rejection of observation (4d rule), Accuracy and precision, Significant figures and their uses. Data manipulation using One-way ANOVA and Prism.

2. Hands on training on the followings:

a. Solvent extraction using Soxhlet apparatus.
b. Distillation techniques: Vacuum distillation, Steam distillation, Azeotrophic distillation, and Fractional distillation.
c. Chromatography: Gas chromatography, Liquid chromatography, Adsorption chromatography, Column chromatography, Flash chromatography, Ion chromatography, High performance liquid chromatography.
d. Measurement of Chemical Oxygen Demand.
e. Thermogravimetric analytical technique and differential scanning calorimetry.
f. Reaction methods: Reflux, Monowave, Microwave, Sonication, Solid phase synthesis, Photolysis/photochemical reactions.
g. Schlenk's technique for handling reaction in inert environment.
h. Preparation, characterization and catalytic applications of nanoparticles.
i. Detection of trace elements (in ppm/ppt) using ICP-OES and AAS.
j. Spectrophotometric and fluorometric based experiments.

Text book:

1) D. A. Skoog, D. M. West and F. J. Holley, *Fundamentals in Analytical Chemistry*, 5th Edn, Saunders, Philadelphia, 1988.
2) D. Harvey, *Modern Analytical Chemistry* (1st Edn), 2000
3) *Nanoparticles and Nanostructured Films: Preparation, Characterization, and Applications*, J. H. Fendler (Ed), Willey, 1998.
5) F. Fox, P.L.H. McSweeney (Eds.), *Advanced Dairy Chemistry*, Vol. 1: Proteins (3rd ed.), Kluwer Academic, Dordrecht, the Netherlands (2003).

Third Semester **CHE-CC-600** **Credits: 4**

ORGANIC CHEMISTRY - III

Unit 1: Application of Spectroscopy

(a) ***Infrared Spectroscopy:*** Identification of organic compounds using characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines and carbonyl compounds (ketones, aldehydes, esters, amides, acid anydrides, lactones, lactams, conjugated carbonyl compounds); Effects of H-bonding and solvent effect on vibrational frequency.

(b) ***Mass Spectroscopy:*** Basic concepts of Mass spectrometry; Structure determination from Mass fragmentation of common organic compounds; McLafferty rearrangements, nitrogen rule, isotope rule.

(c) ***Nuclear Magnetic Resonance Spectroscopy:*** Approximate chemical shift values of carbon- and heteroatom bonded protons; deuterium exchange; chemical and magnetic equivalence; first order and non-first order spectra; Shift reagents; Karplus curve, variation of coupling constant with dihedral angle; ^{13}C-NMR Spectroscopy: Basic concept of ^{13}C-NMR and its chemical shift (aliphatic, olefinic, alkynes, aromatic, hetero-aromatic, carbonyl carbon) values for structure determination.

Unit 2: ***Heterocycles:*** Hantzsch-Widman nomenclature for monocyclic, fused and bridged heterocycles; concept, property, and synthesis of aziranes, oxiranes; azetidines, oxetanes; pyrazole, isoxazole; imidazoles, thiazoles and oxazoles, indole; quinolines, isoquinolines, carbazoles, pteridines, azepines, diazepines.

Unit 3: ***Name reactions:*** Concept, stereochemical aspect and application of Mukaiyama reaction, Henry reaction, Wittig reaction and Horner-Wordwoth- Emmons reaction; Peterson's olefinantion, Prins reaction, Heck reaction, Stille coupling, Suzuki coupling, Chan Lam Coupling, reactions of allylsilane, Biginelli reaction, Hantzsch reaction, Passerini reaction, Ugi reaction, Ring closing metathesis (RCM) - Grubb's reaction, Mitsonobu reaction, Nef reaction, Umpolung effect.

Unit 4: ***(a) Terpenoids:*** Classification of terpenoids (with example); structure and synthesis of abietic acid, caryophyllene, isocaryophyllene, and longifolene.

(b) Alkaloids: Classification of alkaloids (with example); structure and synthesis of strychnine, lysergic acid, nicotine, morphine.

(c) Steroids: Classification of steroids (with example); structure and synthesis of cholesterol, estrogens, and progesterones.

Suggested Books:

[1] R. M. Silverstein, G. C. Basseler & T. C. Morill. Spectroscopic Identification of Organic Compounds, 7th Edn., John Wiley (2005).
[2] Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan, Introduction to Spectroscopy, 5th Edition, Cengage Learning, 2015.
[3] J. A. Joule, K. Mills, Heterocyclic Chemistry, John Wiley & Sons (2010)
[4] M. B Smith, Organic Synthesis (2nd end.), McGraw-Hill, Inc. (2001).
[5] I. L. Finar, Organic Chemistry, Vol. II, 5th edition Pearson (2002).
[6] K. Nakanashi, Natural Products Chemistry, Vols. I and II, Academic Press, New York and London (1974).
[7] D Williams & I. Fleming. Spectroscopic Methods in Organic Chemistry, McGraw Hill (1989).

[8] C. N. Banwell & E. M. McCash. Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, New Delhi (2006).
[9] W. Kemp. Organic Spectroscopy (3rd edn.), McMillan Press Ltd. (1991).
[10] H. O. House. Modern Synthetic Reactions, W. A. Benjamin (1972)
[11] R. Katritzky & C. W. Rees, Comprehensive Heterocyclic Chemistry, Vols. 1-7, Pergamon Press (1984).
[12] J. Alvarez-Builla, J. J. Vaquero (Editor), J. Barluenga, Modern Heterocyclic Chemistry 1st edition Wiley-VCH (2011)
[13] W. Carruthers, Some Modern Methods of Organic Synthesis (4th edn.), Cambridge University Press (2004).
[14] B. M Trost & I Fleming, Comprehensive Organic Synthesis, Vols 1-9, Pergamon (1991).
[15] Katritzky, A. R., Ramsden, C. A., Joule, J. A., and V. V. Zhdankin, Handbook of Heterocyclic Chemistry, 3rd edition, Pergamon Press (2010).
[16] T. L. Gilchrist. Heterocyclic Chemistry (2nd edn.), Longman Scientific & Technical Publicns. (1992).

Third Semester **CHE-CC-601** **Credits: 4**

PHYSICAL CHEMISTRY - IV (PRACTICAL)

A. Students are to perform eight experiments from the following list:

1. Determination of order of reaction, rate constant and energy of activation for saponification of an ester by NaOH, conductometrically.
2. Determination of critical micellar concentration (CMC) of sodium lauryl sulphate from the measurement of conductivities at different concentrations.
3. Determination of strengths of halides in a mixture, potentiometrically.
4. Determination of pH of buffer solutions and hence to calculate the E_0 of quinhydrone electrode.
5. Verification of Beer-Lambert's law and determination of pKa of an indicator, spectro-photometrically.
6. Spectrophotometric determination of pKa of an indicator in micellar and microemulsion media.
7. Determination of partial molar volume of a solute in solution.
8. Determination of the stability constant of the complex formed between Cu(II) ions and 5-sulphosalicylic acid between pH 3-5 by colorimetric method and hence to calculate thefree energy of formation of the complex.
9. Determination of specific rotation of sucrose and rate constant of its hydrolysis using a polarimeter.
10. Determination of coordination number of Cu^{2+} in copper-ammonia complex by partition method.
11. To study the kinetics of iodination of acetone.
12. Determination of the acidic and basic dissociation constants of an amino acid and hence its isoelectric point.
13. To study the phase diagram of three component system.
14. Determination of solubility product for sparingly soluble salt.

B. Experiments based on Fluorescence spectroscopy, Dynamic Light Scattering, TGA-DSC.

Textbooks

1. D. P. Shoemaker, C. W. Garland & J. W. Nibler. *Experiments in Physical Chemistry*, 5th Ed., McGraw Hill Pub., 1989.
2. V. D. Athawala & P. Mathur. *Experimental Physical Chemistry*, New Age International. Publishers, 2001.

Third Semester **CHE-CC-602** **Credits: 4**

INORGANIC CHEMISTRY – III

Unit 1: ***Organometallic Chemistry***

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, Ligands in organometallic chemistry; Synthesis, bonding and reactivity of Metal-alkyl, -alkene, -alkyne, -allyl, -carbene complexes, Agostic interaction, Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples; Catalytic applications: Oxidative addition, Reductive elimination, Hydroformylation (Oxo process), Wacker oxidation (Pd-catalysed), Polymerization of olefins, Ziegler-Natta catalyst**.**

Unit 2: ***Bioinorganic Chemistry***

Essential and trace elements in biological systems, biologically important compounds amino acids, proteins, nucleotides, carbohydrates and lipids, Bioenergetic principle and role of ATP and ADP; Biological membranes; mechanism of ion transport across membranes, ionophores; channel and pump; O_2-uptake proteins: haemoglobin, myoglobin, hemerythrin and hemocyanin, structure, function and model study. Electron transport protein: Fe-S proteins (Rubredoxin and ferredoxins), cytochromes, Metal ions transport and storage proteins: ferritin, transferin, ceruloplasmin.

Unit 3: ***Metal carbonyls, clusters and Metal-metal multiple bond***

Synthesis, structure and reactivity of metal carbonyls; Metal cluster: Low nuclearity and high nuclearity carbonyl clusters; Boron clusters: Structure and bonding of boranes and Lipscomb's topology, styx system of numbering, nomenclature; Synthesis and structure of carboranes, metalloboranes, metallocarboranes; Skeletal electron counting, Wade's rule. Metal-metal multiple bonds, quadruple bond, structures and bonding (MO).

Unit 4: ***Inorganic Supramolecular Chemistry***

Origin of supramolecular chemistry. Concepts and terminology of supramolecular chemistry. Types of supramolecular interactions (Hydrogen bonding, van der Waal's interaction, π-stacking, CH-π, anion-π interaction). Supramolecular chemistry in inorganic perspective: Inorganic crystal engineering and design principle of metal organic framework (MOF) and inorganic-organic hybrid material. Application of supramolecular chemistry in catalysis, drug delivery, and recognition/sensing.

Text Books

1. C. Elschenbroich, *Organometallics* (3rd edn.), Wiley-VCH Publication (2006).
2. R. C. Mehrotra & A. Singh, *Organometallic Chemistry: A Unified Approach* (2nd edn.), New Age International (2000).
3. S. J. Lippard & J. M. Berg, *Principles of Bio-Inorganic Chemistry*, Panima Publ. Corpn. (2005).
4. J. W. Steed & J. L. Atwood. *Supramolecular Chemistry*, John Wiley (2002).

Reference Books

1. Yamamoto, *Organo Transition Metal Chemistry*, Wiley (1986).
2. R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals* (4th edn.), John Wiley (2005).
3. Gautam R Desiraju, J. J Vittal, A. Ramanan, *Crystal Engineering: A Textbook* (1st Edn.) World Scientific Publishing Company (2011)

Third Semester **CHE-DSEC-603** **Credits: 4**

INSTRUMENTAL TECHNIQUES IN INORGANIC CHEMISTRY

Unit 1: ***EPR and NMR Spectroscopy:*** Principle, instrumentation, representation of EPR spectrum, line width, hyperfine splitting, magnetically equivalent and nonequivalent sets of nuclei, g-anisotropy, spectra of simple organic free radicals: Spectra of transition metal complexes, zerofield splitting, application: determination of oxidation state of metal ion in samples. NMR spectroscopy; Applications of ^{31}P, ^{19}F, ^{119}Sn and ^{195}Pt NMR spectroscopy in the structural assessment of inorganic compounds.

Unit 2: (a) ***IR, UV-vis and Fluorescence Spectroscopy:*** Structural studies of coordination compounds using IR and Raman spectroscopy; Basics of UV-vis and emission spectroscopy. d-d and charge transfer spectra. Stokes shift, fluorescence phosphorescence, quantum yield.

(b) ***Mössbauer Spectroscopy***: Principles, isomer shift, quadrupole effect of magnetic field, applications of Mössbauer Spectroscopy involving iron and tin compounds.

Unit 3: Other Techniques

(a) X-ray Crystallography**:** Principle and Instrumentation, Crystal systems, Symmetry-operations, point groups, space groups, Techniques of single Crystal growth. Structure determination by single-crystal X-ray crystallography; Elements of powder diffraction method.

(b) Electrochemistry**:** Principles, instrumentation and applications of cyclic voltametry.

(c) Thermonalytical methods**:** Principles, instrumentation and applications of thermoanalytical methods, *viz.* TGA, DTA and DSC.

Unit 4: Exercises on the structure elucidation by joint applications of the following techniques: NMR, Mass spectrometry, X-ray Diffraction methods

Exercises on the spectroscopic study: UV-Vis, Fluorescence, IR, Mossbauer, EPR spectroscopy.

Text Books

1. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, (6^{th} edn.), John Wiley (2008).
2. R. V. Parish, *NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry*, Ellis Horwood, New York (1990).
3. J. A. Iggo, *NMR Spectroscopy in Inorganic Chemistry*, OUP Oxford (2000)
4. G. H. Stout and L. H. Jensen, *X-ray Structure Determination: A Practical Guide*, The McMillan Company, New York (1968)
5. F. Marken, A. Neudeck A. M. Bond, *Electroanalytical Methods*, Chapter III, 51–97 (2005)

Reference Books

1. R. S. Drago. *Physical Methods in Chemistry*, Saunders College Publishers (1977).

Third Semester **CHE-DSEC-604** **Credits: 4**

Organic Chemistry IV

RESEARCH TOOLS FOR ORGANIC CHEMISTRY

Unit 1: Working principles, sample preparation, instrumentation of ^{1}H, ^{13}C and HRMS.

Unit 2: Structure elucidation of some simple and complex organic molecules by the analysis of FT-IR, ^{1}H, ^{13}C and mass data.

Unit 3: Working principles, sample preparation, instrumentation of GC, GC-MS, HPLC, MS-Ms and MALDI-TOF.

Unit 4: Working principles, sample preparation, instrumentation of SEM, TEM, PXRD, XPS, ICP-AES or ICP-OES, BET measurements

Text Book

1. R.M. Silverstein, Go Clayton Bassler and C. Morril, *Spectrometric Identification of Organic Compounds*, 5th Ed,-John Wiley & Sons, 1991. ..
2. W. Kemp, *Organic Spectroscopy*, 3rd Ed, ELBS, 1991
3. K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part A&B; John Wiley and Sons Inc., 6th Ed, 2009.
4. P. I. Haines, Thermal *Methods of Analysis-Principles, Applications and Problems*, Blackie Academic & Professional, 1st Ed, 1995.

Third Semester **CHE-DSEC-605** **Credits: 4**

PHYSICAL CHEMISTRY – V

RESEARCH TOOLS IN PHYSICAL CHEMISTRY

Unit 1: Fluorescence Spectroscopy

Basic concept: Origin of molecular fluorescence; intensity and spectra; Quantum yield; Steady state and time-resolved techniques; Experimentally measured parameters; Factors affecting fluorescence spectra; fluorescence quenching and applications; Monitoring excited state properties: Radox behavior and dipole moment; Excited state processes studied through fluorescence - charge transfer, proton transfer, energy transfer etc. Biological applications - some selected examples.

Unit 2: Photoelectron Spectroscopy

Basic principles, photoelectron spectra of simple molecules, X-ray photoelectron spectroscopy (ESCA), Auger electron spectroscopy. Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems. Dynamic Light Scattering: Principles and Applications (determination of Hydrodynamic diameter and ζ-potential.)

Unit 3: Numerical Analysis

Curve fitting by least square principle; Newton–Raphson iterative methods for solving non-linear equations; Interpolation, Numerical differentiation and integration, trapezoidal method, Simpson's 1/3 rule; Runge-Kutta method for solving differential equations.

Unit 4: Computational Chemistry

(A) Ab-initio methods: Hatree-Fock (HF) and post-HF methods; Density functional theory; semi-empirical methods.

(B) Applications of computational chemistry: geometry optimization; energy and frequency calculations; thermochemistry, kinetics, spectroscopic properties; molecular dynamics etc. Computational chemistry software: GAUSSIAN, GAMESS, GROMACS, AUTO DOCK.
Visualization softwares: Gaussview, pymol, VMD, Avogadro.

(C) Hands-on training with computers on selected chemical problems for unit 4.

Text Books

1. J.R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd ed., Springer, Boston, USA, 2006.
2. E. Balagurusamy, *Computer Oriented Statistical and Numerical Methods*, Macmillan IndiaLtd. 2000.
3. Christopher J. Cramer, *Essentials of Computational Chemistry*, 2nd Ed., Wiley, 2002.
4. K. Atkinson, An introduction to numerical analysis 2nd Ed. Wiley, 2007.

Reference Books

1. E. Kreyszig. *Advanced Engineering Mathematics*, 5th edn., Wiley Eastern Ltd.,1985.
2. E.W. Cheney, D.R. Kincaid, *Numerical Mathematics and Computing*, Cengage Learning, 2007.

Fourth Semester **CHE-DSEC-606** **Credits: 4**

Research Project