DEPARTMENT OF CHEMISTRY
NORTH-EASTERN HILL UNIVERSITY
SHILLONG 793 022

M. Sc. CHEMISTRY SYLLABUS

CHOICE BASED CREDIT SYSTEM (CBCS)

(*PROPOSED REVISED SYLLABUS: 2016*)

M. Sc. CHEMISTRY COURSE STRUCTURE (*Revised Proposal*)

FIRST SEMESTER

Course number	*Course name*	Credits	Marks	Total
CHE -C-101	Inorganic Chemistry-I	**4**	100	
CHE -C-102	Organic Chemistry-I	**4**	100	**18**
CHE -C-103	Physical Chemistry-I	**4**	100	
CHE -C-104	Laboratory Course-I (Organic Chemistry)	**6**	150 450	

SECOND SEMESTER

Course number	*Course name*	Credits	Marks	Total
CHE -C-201	Inorganic Chemistry-II	**2**	50	
CHE -C-202	Organic Chemistry-II	**2**	50	
CHE -C-203	Physical Chemistry-II	**2**	50	
CHE -C-204	Laboratory Course-I (Inorganic Chemistry)	**6**	150	**18**
CHE -O-205	Computer Programming and Applications in Chemistry (Open Choice)	**2**	50	
CHE -O-206	Chemistry of Polymers and Biomolecules (Open Choice)	**4**	100	

THIRD SEMESTER

Course number	*Course name*	Credits	Marks	Total
CHE-C-301	Inorganic Chemistry-III	**2**	50	
CHE -C-302	Organic Chemistry-III	**2**	50	
CHE -C-303	Physical Chemistry-III	**2**	50	
CHE -C-304	Laboratory Course-I (Physical Chemistry)	**6**	150	**18**
CHE -O-305	Photochemistry (Open choice)	**2**	50	
CHE -O-306	Selected Topics in Inorganic Chemistry (Open Choice)	**4**	100	

FOURTH SEMESTER

Course number	*Course name*	Credits	Marks	Total
CHE -C-401	Inorganic Chemistry-IV	**4**	100	
CHE -C-402	Organic Chemistry-IV	**4**	100	**18**
CHE -C-403	Physical Chemistry-IV	**4**	100	
CHE -C-404	Project Work	**6**	150	

First Semester **CHE-C-101** **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.

Unit 2
(a) Stereochemistry and Bonding: LCAO-MO theory for homonuclear and heteronuclear diatomic molecules; orbital symmetry and overlap; Walsh diagrams; electronegativity (Pauling, Mulliken and Allred-Rochow methods); and polarity of bonds; review of VSEPR model and the use of outer d-orbitals.
(b) 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.

Unit 3 ***Magnetochemistry***
Brief review of different types of magnetic substance and magnetic behaviour, measurement of magnetic susceptibility using Gouy's and Faraday's methods, 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 superexchange mechanism.

Unit 4 ***Electronic Structure of Transition Metal Complexes***
Electronic absorption spectra of octahedral and tetrahedral complexes, Orgel diagrams, Tanabe- Sugano diagrams, calculation of Dq, B and ß values, selection rules, band intensities and band widths, spectra of high-spin octahedral and tetrahedral complexes of d1 to d9 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-C-102** **Credits: 4**

ORGANIC CHEMISTRY – I

Unit 1

***Stereochemistry*:** Configuration nomenclature; Axial and planar chirality and helicity; Topicity and prostereoisomerism; Racemic modification and optical purity; Conformational analysis of acyclic, cyclic, heterocyclic and steroidal systems; Effects of conformation on reactivity. Concept of regioselectivity, stereospecificity and stereoselectivity.

Unit 2

***Aromaticity and reaction mechanisms*:** Concept and application of aromaticity, Aromaticity in benzenoid and non-benzenoid compounds, *n*-annulenes, heteroannulenes, fullerenes, cryptates. Machanism, 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, aldol condensation (Zimmerman and Evans models).

Unit 3

Photochemistry: Photochemistry of alkenes and carbonyl compounds; Photooxygenation; Photochemistry of aromatic compounds; Photochemical isomerisation, addition and substitution; Photo-Fries rearrangement of ethers and anilides; Barton reaction, Hoffmann-Loefller-Freytag reaction, di-π-methane rearrangement; Singlet molecular oxygen reactions; photo-cleavages.

Unit 4

***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 (*hv* 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.

Text Books

1. D. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edn, New Age International (1994).
2. *March*'s *Advanced Organic Chemistry: Reactions, Mechanisms and Structure* (6th edn.), Wiley Student Edition, John Wiley & Sons Asia Pte. Ltd. (2006).
3. P. S. Kalsi. *Stereochemistry, Conformation and Mechanism* (7th edn.), New Age (2008).
C. Depuy & O. L. Chapman. *Molecular Reactions and Photochemistry*, Prentice-Hall of India (1975).

Reference Books

1. F. A. Carey & R. J. Sanburg. *Advanced Organic Chemistry*, Part A and B, 5th edition (2008).
2. R. B Woodward & R. Hoffman, *Conservation of Orbital Symmetry*; Verlag-Chemie Academic Press (1970).
3. I. Fleming. *Frontier Orbital Theory and Organic Reactions*, John Wiley & Sons (1976).
4. A. P. Marchand & R. E. Lehr, *Pericyclic Reactions*, Academic Press (1977).
5. Subrata Sengupta, Basic Stereochemistry of Organic Molecules, 1st Edn., Oxford Univ Press, (2014)

First Semester **CHE-C-103** **Credits: 4**

PHYSICAL CHEMISTRY – I

Unit 1 ***Quantum Mechanics and its Applications***

Introduction; operators and related theorems; uncertainty principle; postulates; properties of wave functions; Schrodinger equation; energy Eigen value equation; equation of motion and constant of motion.

Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential and tunnelling, hydrogen atom.

Approximate methods: Variation theorem and 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; non-crossing rule and correlation diagram; hybridization; Huckel MO treatment for conjugated π-electron systems.

Unit 3 ***Adsorption and Aggregation***

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; Adsorption on solids: Langmuir isotherm, BET 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.

Unit 4 ***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, thermodynamics of Schottky and Frenkel defect formation.

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

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

Text Books

1. D. A. McQuarrie*, Quantum Chemistry*, Viva Books Pvt Ltd (2010)
2. Y. Moroi *Micelles: Theoretical and Applied Aspects*, Plenum (2003).
3. A. R. West *Solid State Chemistry and its Applications*, John Wiley (2001).

Reference Books

1. P. W. Atkins *Molecular Quantum Mechanics*, Oxford University Press (2007)
2. R. McWeeny *Coulson's Valence*, ELBS (2000).

First Semester **CHE- C-104** **Credits: 6**

LABORATORY COURSE – I
(ORGANIC CHEMISTRY)

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: Solasodine, caffeine, nicotine, piperine, rosine, carotenoids, curcumin, and citral.

3. Organic preparations, purification by recrystallization/chromatography and characterization by m.p., IR, UV, ^{1}HNMR and ^{13}CNMR and MS: At least eight preparations involving the following representative reactions-
   a. Esterification and saponification
   b. Oxidation (per acid, chromic acid, Mn(Vll)
   c. Hydride reduction or hydrogenation
   d. Nucleophilic substitution
   e. Cycloaddition reaction
   f. Biginelli reaction
   g. Condensation reaction
   h. Preparation of dyes
   i. Aromatic electrophilic substitution
   j. Synthesis of bis-coumarin
   k. Synthesis Pyranopyrazole
   l. Synthesis of bis-indolyl derivatives

4. Ferrite, nickel and Copper nanoparticle synthesis, characterization (UV, IR, SEM, TEM, DLS) and application.

5. Qualitative Analysis of Binary Mixtures (only two)

Text Books

1. A. I. Vogel. *Practical Organic Chemistry* (5th edn.), Longman Group Ltd. (1989).
2. C N R Rao, A Muller, A K Cheetham, *The Chemistry of Nanomaterials: Synthesis, Properties and Applications*, 2 Volumes, Wiley-VCH (2004).

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).
3. R. K. Bansal. *Laboratory Manual of Organic Chemistry* (3rd edn.), Wiley-Eastern (1994).
4. R. G. Brewster & W.E. Mcwedn. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).

Second Semester **CHE-C-201** **Credits: 2**

INORGANIC CHEMISTRY – II

Unit 1 ***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 bond, quadruple bond, structures and bonding (MO).

Unit 2 ***Reaction Mechanism of Transition Metal Complexes***

Energy profile of reactions, 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 non-rigidity and fluxional molecules.

Text Books

1. J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, *Principles, Structure and Reactivity* (1st impression), Pearson Education (2006).
2. F. A. Cotton, G. Wilkinson, C.A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry* (6th edn.), John Wiley (1999).
3. N. N. Greenwood & A. Earnshaw. *Chemistry of the Elements*, Pergamon Press (1984).
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. T. Moeller. *Inorganic Chemistry: A Modern Approach*, John Wiley (1982).

Second Semester **CHE-C-202** **Credits: 2**

ORGANIC CHEMISTRY – II

Unit 1: *Catalysts and Reagents*: Concept, stereochemical aspect and application of catalytic hydrogenation, hydride reduction, hydroboration, dissolving metal reductions. carbonyl reduction with hydrazine derivatives. Concept, stereochemical aspect and application of metallic and non-metallic oxidants, such as PCC, PDC and Collin's reagent, Swern oxidation, IBX, Dess-Martin periodinane; MnO2, Ag2CO3 on celite, peracids, metal/alkyl hydroperoxides, Sharpless asymmetric epoxidation and asymmetric dihydroxylation, dioxiranes, $I2/Ag^{+}$; periodates, LTA, SeO2, etc.

Unit 2: *Reactive Intermediates*: Concept, generation, stereochemical aspects, and synthetic applications (important name reactions) of carbenes, nitrenes, arynes and free radicals.

Textbooks

1. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure (6^{th} edn.), Wiley Student Edition, John Wiley & Sons Asia Pte. Ltd. (2006).
2. F. A. Carey & R. J. Sundberg. *Advanced Organic Chemistry* Part B, Plenum Press, 5^{th} edition (2008).
3. M. B Smith. *Organic Synthesis* (2^{nd} end.), McGraw-Hill, Inc. (2001).
4. T. L. Gilchrist & C. W. Rees, Carbenes, Nitrenes and Arynes, Nelson, London (Reprinted 2008).

Reference Books

1. W. Carruthers. *Some Modern Methods of Organic Synthesis* (4^{th} edn.), Cambridge University Press (2004).
2. B. M. Trost & I Fleming. *Comprehensive Organic Synthesis*, Vols 1-9, Pergamon (1991).
3. H. O. House. *Modern Synthetic Reactions*, W. A. Benjamin (1972).

Second Semester **CHE-C-203** **Credits: 2**

PHYSICAL CHEMISTRY - II

Unit 1 ***Rotational and Vibrational and Electronic Spectroscopy***
Introduction: Interaction of light with matter, mechanism of absorption & 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. 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.

Unit 2 ***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. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th edn., Tata McGraw-Hill, New Delhi (2002).
2. D. A. McQuarrie and J.D. Simon, *Physical Chemistry*, VIVA Students Ed. (2003)

Reference Books

1. J. D. Graybeat. *Molecular Spectroscopy*, McGraw-Hill International Edition (1988).

Second Semester **CHE-C-204** **Credits: 6**

LABORATORY COURSE – II
(INORGANIC CHEMISTRY)

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 7 preparations are to be completed by turn):

I. Tris(acetylacetonato) iron(III)
II. Tris(acetylacetonato)manganese(III)
III. Reinecke salt
IV. Tris(oxalate) manganese(III)
V. Tetrapyridinesilver(II)peroxidisulphate
VI. Bis(N,N-diethyldithiocarbamato)nitrosyliron(I)
VII. Optical isomers of tris(ethylenediamine)cobalt(III)chloride
VIII. Linkage isomers of nitro and nitritopentamminecobalt(III) chloride
IX. Hydridochlorocarbonyl tris(triphenylphosphine)ruthenium(II)
X. Tris(2,2′-bipyridine)ruthenium(II) perchlorate
XI. $[(p\text{-(cymene)}RuCl_2]_2$

3. Synthesis and characterization of metal Schiff base complex.

Characterization includes microanalysis, magnetic susceptibility 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-O-205** **Credits: 2**

COMPUTER PROGRAMMING AND APPLICATIONS IN CHEMISTRY

Unit 1 ***Introduction to FORTRAN Language and Programming***

Programming tools, Constants, variables and expressions, input and output statements, format specifications, control statements, nesting of loops, arrays and subscripted variables, functions and subroutines.

Unit 2 ***Numerical Analysis and Computational Methods in Chemistry***

(A) 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;

(B) Electronic structure calculations using computational chemistry software, GAUSSIAN, GAMESS etc: geometry optimisation; energy and frequency calculations; thermo-chemistry analysis; visualisation.

(Hands on training with computers on selected chemical problems based on the numerical techniques of Units 1 & 2).

Text Books

1.W. E. Mayo & M. Chiakala, *Programming with FORTRAN 77*, Schaum's Outline Series,New Delhi (1995).
2. E. Balagurusamy, *Computer Oriented Statistical and Numerical Methods*, Macmillan IndiaLtd. 2000).
3. A. C. Norris, *Computational Chemistry: An Introduction to Numerical Methods*, John Wiley, New York (1981).

Reference Books

1. E. Kreyszig. *Advanced Engineering Mathematics* (5th edn.), Wiley Eastern Ltd. (1985).
2. C. Xavier. *Programming in Fortran 77 and Numerical Methods*. Asian Books (1998).
3. E.W. Cheney, D.R. Kincaid, *Numerical Mathematics and Computing,* Cengage Learning (2007).

Second Semester **CHE-O-206** **Credits: 4**

CHEMISTRY OF POLYMERS AND BIOMOLECULES

Unit l

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.

Unit 2

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 3

Co-Enzyme**:** Structure & function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid and vitamin B12 in biological processes.
Nucleic acids: Primary, secondary and tertiary structure of DNA; DNA replication and heredity; Structure and function of mRNA, tRNA and rRNA. Role of ATP in biological processes.

Unit 4

Drug-development**:** Concept of drug, lead compound, prodrugs and soft drugs; ADME, Structure-activity relationship (SAR), quantitative structure-activity relationship (QSAR); Theories of drug action, drug metabolism. Concept, classification, SAR and mode of action of Antibiotics (penicillin), Anticancer, Antimalarial, sedatives and Hypnotices drugs. Synthesis of diazepam, barbiturates, thiopental sodium, chloroquine and pamaquine.

Text Books

1. A. L. Lehninger. *Biochemistry*, 8th edition, Kalyani Publishers (2008).
2. G. Thomas. *Medicinal Chemistry: An Introduction*, 2nd Edition, Wiley (2007).
3. M. S. Bhatnagar. *A textbook of polymer chemistry, Vol (I-III)*: S. Chand and Company (2004).
4. J. W. Steed and J. L. Atwood. *Supramolecular Chemistry*: Willy Reprinted (2002).

Reference Books

1. Burger. *Medicinal Chemistry and Drug Discovery*, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
2. Goodman & Gilman. *Pharmacological Basis of Therapeutics*, McGraw-HilI (2005).
3. S. S. Pandeya & J. R. Dimmock. *Introduction to Drug Design*, New Age International.(2000).
4. Graham & Patrick. *Introduction to Medicinal Chemistry* (3rd edn.), OUP (2005).
5. D. Lednicer. *Strategies for Organic Drug Synthesis and Design*, John Wiley (1998).
6. T. Nogrady, D.F. Weaver *Medicinal Chemistry* Oxford University Press (2005).
7. D. Smith, D. Walker, H. van de Waterbeemd *Pharmacokinetics and Metabolism in Drug Design*, WILEY-VCH (2001)

Third Semester **CHE-C-301** **Credits: 2**

INORGANIC CHEMISTRY – III

Unit 1 ***EPR and NMR Spectroscopy***

Electron Paramagnetic Resonance Spectroscopy: Principle, instrumentation, representation of EPR spectrum, X-band and Q-band spectra, line width, hyperfine splitting, magnetically equivalent and nonequivalent sets of nuclei, g-anisotropy, spectra of simple organic free radicals: expected number of lines, intensities. Spectra of transition metal complexes, metal hyperfine anisotropic spectra, zero-field splitting, application: determination of oxidation state of metal ion in samples.

Nuclear magnetic resonance spectroscopy: Applications of ^{31}P, ^{19}F, ^{119}Sn and ^{195}Pt NMR spectroscopy in the structural assessment of inorganic compounds.

Unit 2 ***Infrared and Raman Spectroscopy***

Structural studies (involving IR and Raman spectroscopy) of coordination compounds containing the following molecules/ions and ligands - NH_3, H_2O, OH^-, SO_4^{2-}, CN^-, SCN^-, NO_2^-.

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

X-ray Crystallography: X-ray diffraction and Bragg's law; Crystal systems and symmetry, point groups, stereographic projection of 32 point groups and space groups-Hermann–Mauguin notations, space group in triclinic and monoclinic system; Primitive and non-primitive unit cells; Symmetry elements: isogonal symmetry groups and reciprocal lattice. Crystal growing; X-ray-instrumentation Data collection, data reduction, refinement and structure solution.

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)

Reference Books

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

Third Semester **CHE-C-302** **Credits: 2**

ORGANIC CHEMISTRY – III

Unit 1

***(a) Infrared Spectroscopy*:** Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines; Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acid anydrides, lactones, lactams, conjugated carbonyl compounds); Effects of H-bonding and solvent effect on vibrational frequency, extension to various organic molecules for structural assignment.

***(b) Mass Spectroscopy*:** Mass spectral fragmentation of organic compounds, common functional groups; molecular peak, McLafferty rearrangements, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Unit 2

***(a) Nuclear Magnetic Resonance Spectroscopy*:**
Approximate chemical shift values of various chemically non-equivalent protons and correlation to protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic); Protons bonded to other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, SH); Chemical exchange, effect of deuteration; complex spin-spin interaction between two, three, four and interacting nuclei (first order spectra); Complex interaction, virtual coupling, stereochemically hindered rotation, Karplus curve, variation of coupling constant with dihedral angle, nuclear magnetic double resonance, simplification of complex spectra using shift reagents, Fourier transform technique and nuclear Overhauser effect (NOE).

***(b) C-13 NMR Spectroscopy*:**
Chemical shift (aliphatic, olefinic, alkynes, aromatic, hetero-aromatic, carbonyl carbon); Coupling constants, two-dimensional NMR spectroscopy, NOESY, DEPT and INEPT terminologies.

(c) Applications of IR, NMR and Mass spectroscopy for structure elucidation of organic compounds.

Textbook

R. M. Silverstein, G. C. Basseler & T. C. Morill. *Spectroscopic Identification of Organic Compounds*, 7th Edn., John Wiley (2005).
Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan, *Introduction to Spectroscopy*, 5th Edition, Cengage Learning, 2015.
P.S. Kalsi, Stereochemistry conformation and mechanism (7th Edn), New Age International (2008).

References

1. D Williams & I. Fleming. *Spectroscopic Methods in Organic Chemistry*, McGraw Hill (1989).
2. C. N. Banwell & E. M. McCash. *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill, New Delhi (2006).
3. W. Kemp. *Organic Spectroscopy* (3rd edn.), McMillan Press Ltd. (1991).

Third Semester **CHE-C-303** **Credits: 2**

PHYSICAL CHEMISTRY – III

Unit 1 ***Chemical Thermodynamics***

Thermodynamics of ideal and non-ideal gases and solutions, Criteria of thermodynamic equilibrium - chemical potential; concept of fugacity, standard state of real gases, the relation between fugacity and pressure; Partial molar quantities, partial molar volume and its determination, thermodynamics of mixing; Activity and activity coefficients.

Unit 2 ***Statistical Thermodynamics: Theory and Applications***

(A) Different types of ensembles, ensemble averaging, distribution law (Boltzmann statistics), partition function and thermodynamic parameters; relation between molecular and molar partition functions, 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, equilibrium constant in terms of 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

Text Books

1. P. W. Atkins & J. de Paula, Physical Chemistry (8th edn.), OUP (2006).
2. D. A. McQuarrie, Statistical Mechanics, Viva Books Pvt. Ltd., New Delhi (2003).

References

2. T. L. Hill, *Statistical Mechanics*, McGraw Hill (1989).
3. K Huang, *Statistical Mechanics*, OUP (2006).

Third Semester **CHE-C-304** **Credits: 6**

LABORATORY COURSE – III

(PHYSICAL CHEMISTRY)

A. Students are to perform twelve 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, spectrophotometrically.
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 edn.), McGraw Hill (1989)
2. V. D. Athawala & P. Mathur. *Experimental Physical Chemistry*, New Age International. Publishers (2001).

Third Semester **CHE-O-305** **Credits: 2**

PHOTOCHEMISTRY

Unit 1 ***Principles of Photochemistry***

Laws of photochemistry, quantum yield, nature of changes on electronic excitation, Potential energy diagram, Absorption band shape and Franck-Condon Principle, Emission Spectra, Environmental effects on absorption and emission properties, Excited state dipole moment, Redox potential and acidity constants of aromatic acids.

Types of photophysical pathways, Radiationless transitions, Fluorescence emission, Triplet state and phosphorescence emission, Fluorescence quenching, Stern-Volmer equation, Concentration quenching and excimer formation, Quenching by foreign substrates, Exciplex formation.

Unit 1 ***Applications of Photochemistry***

Role of photochemical reactions in biochemical processes, origin of life, photosynthesis, mechanism of vision.

Photo-reduction and photo-oxidation related reactions, cycloaddition reaction, chemiluminescence, transition metal complexes.

Fluorescence sensing: Mechanism of sensing, sensing techniques based on (i) collisional quenching (ii) energy transfer (iii) electron transfer. Examples of (i) pH sensors (ii) glucose sensors and (iii) protein sensors.

Text Books

1. N. J. Turro V. Ramamurthy, J.C. Scaiano*, Principles of Molecular Photochemistry An Introduction* University Science Books (2009).
2. J. R. Lakowicz. *Principles of Fluorescence Spectroscopy*, Springer (2006).

Reference Books

1. J.B. Buirks. *Photophysics of Aromatic Molecules*, Wiley-Interscience (1969).
2. A. Gilbert & J.E. Baggott, *Essentials of Molecular Photochemistry*, Blackwell Scientific, Oxford (1991).

Third Semester **CHE-O-306** **Credits: 4**

SELECTED TOPICS IN INORGANIC CHEMISTRY

Unit 1. ***Basic 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, -carbyne and -carbide complexes, Agostic interaction, Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples; Main group organometallics: Synthesis and reactions of organolithium and organomagnesium compounds; Organometallics of zinc and mercury: preparation, structure, bonding and reactions of aluminum organyls.

Unit 2 ***Basic 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: hemoglobin, 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 ***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, recognition/sensing and material science.

Unit 4 ***Nanomaterials***

General introduction to nanomaterials; Moore's law; synthesis and properties of nanoparticles; Synthesis of nanoparticle semiconductors, nanowires and nanorods; Synthesis, structures and properties of C_{60} and related compounds; Synthesis, structures and applications of single walled (SWNTs), multi-walled (MWNTs) carbon nanotubes; Techniques of synthesis: electroplating and electrophoretic deposition, conversion through chemical reactions and lithography; Thin films: Chemical vapor deposition and Atomic layer deposition techniques; Analysis techniques using spectroscopy and microscopy; Applications of nanomaterials.

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).
5. M. Ratner & D. Ratner, *Nanotechnology: A Gentle Introduction to the Next Big Idea*, Pearson Education (2003).

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. 4. M. Bochmann. *Organometallics-I and II Complexes with Transition Metal-Carbon σ-and π-Bonds*, Oxford Chemistry Primers (1994).
4. Gautam R Desiraju, J. J Vittal, A. Ramanan, *Crystal Engineering: A Textbook* (1st Edn.) World Scientific Publishing Company (2011)

Fourth Semester **CHE-C-401** **Credits: 4**

INORGANIC CHEMISTRY – IV

Unit 1 ***Chemistry of η^3-η^6 cyclic metal analogues***

Chemistry of η^3-η^6 cyclic, sandwich and half-sandwich transition metal complexes. Synthesis and reactions of cyclopentadienyl metal carbonyls, cyclopentadienyl metal hydrides, cyclopentadienyl metal halides, arene metal group complexes, η^6-arene-chromium tricarbonyl in organic synthesis.

Unit 2 ***Catalytic applications of organometallic chemistry***

Terminology in catalysis: TO, TON, TOF; Unique reactions in organometallic chemistry and catalysis: Coordinative unsaturation, Substitution, Oxidative addition, Insertion (migration), Isomerization, Reductive elimination; Catalytic converters; Alkene hydrogenation, Hydroformylation (Oxo process), Carbonylation of olefins, Monsanto's acetic acid synthesis, Wacker oxidation (Pd-catalysed), Polymerization of olefins, Ziegler-Natta catalyst**.**

Unit 3 ***Advanced Bioinorganic Chemistry***

Metalloenzymes: Copper enzymes, superoxide dismutase, cytochrome oxidase; Coenzymes; Molybdenum enzyme: Xanthine oxidase, Nitrate reductase, Sulphate oxidase; Zinc enzymes: carbonic anhydrase, carboxy peptidase; Vitamin B12 and B12 coenzymes; Vanadium containing protein: Amavadin, Vanadium bromo peroxidase; Metal dependent diseases: Wilson's disease, Alzheimer disease; Transition metal complexes as drugs.

Unit 4 ***Inorganic Photochemistry***

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; Application of inorganic photochemistry: Molecular recognition, Sensing, supramolecular chemistry, Photochemical splitting of water, Dye sensitized solar cells.

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. D. M. Roundhill. *Photochemistry and Photophysics of Metal Complexes*, Plenum Press (1990).
5. J. E. Huheey, E. A. Keiter & R. L. Keiter*, Inorganic Chemistry* (4^{th} edn) Prentice Hall (1997)

Reference Books

1. F. A. Cotton & G. Wilkinson, *Advanced Inorganic Chemistry* (5^{th} edn.), John Wiley (1988)
2. C. Cutal & A.W. Adamson, *Comprehensive Coordination Chemistry*, Vol. 1, Editor-in-Chief G. Wilkinson (1985).
3. A.W. Adamson & P.D. Fleischauer. *Concepts of Inorganic Photochemistry*, John Wiley & Sons (1975).
4 P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong. *Shriver and Atkins Inorganic Chemistry*, Oxford University Press (2006).

Fourth Semester **CHE-C-402** **Credits: 4**

ORGANIC CHEMISTRY -IV

Unit 1

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

Unit 2

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 3

Terpenoids and alkaloids: Basic concepts of retrosynthesis, Classification of terpenoids and alkaloids, Structure, Retrosynthesis and Synthesis (including stereoselective) of abietic acid, *cis* juvenile hormone, caryophyllene, isocaryophyllene, longifolene, Strychnine, lysergic acid, reserpine, nicotine, morphine, emitine.

Unit 4

Steroids: Classification of steroids, Structure, Retrosynthesis and Synthesis (including stereoselective) of squalene; Lanosterol and caretonoids; Synthesis of equlenins; Estrogens and total synthesis of non-aromatic steroids (progesterones); Corticosteroids; Degradation of diosgenin to progesterone and its synthesis; Miscellaneous transformations of steroid molecules.

Textbooks

1. J. A. Joule, K. Mills, *Heterocyclic Chemistry*, John Wiley & Sons (2010)
2. M. B Smith, *Organic Synthesis* (2nd end.), McGraw-Hill, Inc. (2001).
3. I. L. Finar, *Organic Chemistry*, Vol. II, 5th edition Pearson (2002).
4. K. Nakanashi, *Natural Products Chemistry*, Vols. I and II, Academic Press, New York and London (1974).

Reference Book

1. R. Katritzky & C. W. Rees, *Comprehensive Heterocyclic Chemistry*, Vols. 1-7, Pergamon Press (1984).
2. J. Alvarez-Builla, J. J. Vaquero (Editor), J. Barluenga, *Modern Heterocyclic Chemistry* 1st edition Wiley-VCH (2011)
3. W. Carruthers, *Some Modern Methods of Organic Synthesis* (4th edn.), Cambridge University Press (2004).
4. B. M Trost & I Fleming, *Comprehensive Organic Synthesis*, Vols 1-9, Pergamon (1991).
5. Katritzky, A. R., Ramsden, C. A., Joule, J. A., and V. V. Zhdankin, *Handbook of Heterocyclic Chemistry*, 3rd edition, Pergamon Press (2010).
6. T. L. Gilchrist. *Heterocyclic Chemistry* (2nd edn.), Longman Scientific & Technical Publicns. (1992).

Fourth Semester **CHE-C-403** **Credits: 4**

PHYSICAL CHEMISTRY – IV

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, Study of rapid reactions: Flow, stopped–flow, Relaxation and NMR techniques.

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 ***Electrochemistry***

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.

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 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. J. O'M Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Plenum, New York (2007).
2. K. J. Laidler, *Chemical Kinetics* (4th Edn.), Pearson Eductions (2007).
3. D. A. McQuarrie and J.D. Simon –*Physical Chemistry*, VIVA Students Ed. (2003)
4. C. Kalidas and M. V. Sanganarayana, *Non-Equilibrium Thermodynamics – Principles and Applications*, Macmillan India (2002).

Reference Book

1. M. J. Pilling and P. W. Seakins. *Reaction Kinetics*, NP (1995).
2. I. Prigogine. *Introduction to Thermodynamics of Irreversible Processes*, Interscience (1960).