A Satyam Roychowdhury initiative

TECHNO INDIA GROUP

SNU

SISTER NIVEDITA UNIVERSITY

TWO YEAR SYLLABUS

OF

Master of Science in

CHEMISTRY

Vice-Chancellor,

Sister Nivedita University

Subject Expert

Raj K Datta

Chief General Manager - Product Development, Technical Support & QA

Haldia Petrochemicals Limited

Industry Expert

Head of the Department,
Chemistry, SNU

Curriculum for M.Sc. CHEMISTRY

SCHOOL OF NATURAL SCIENCE

M.Sc. Chemistry

Credit Definition

Type	Duration (in Hour)	Credit
Lecture (L)	1	1
Tutorial (T)	1	1
Practical (P)	2	1

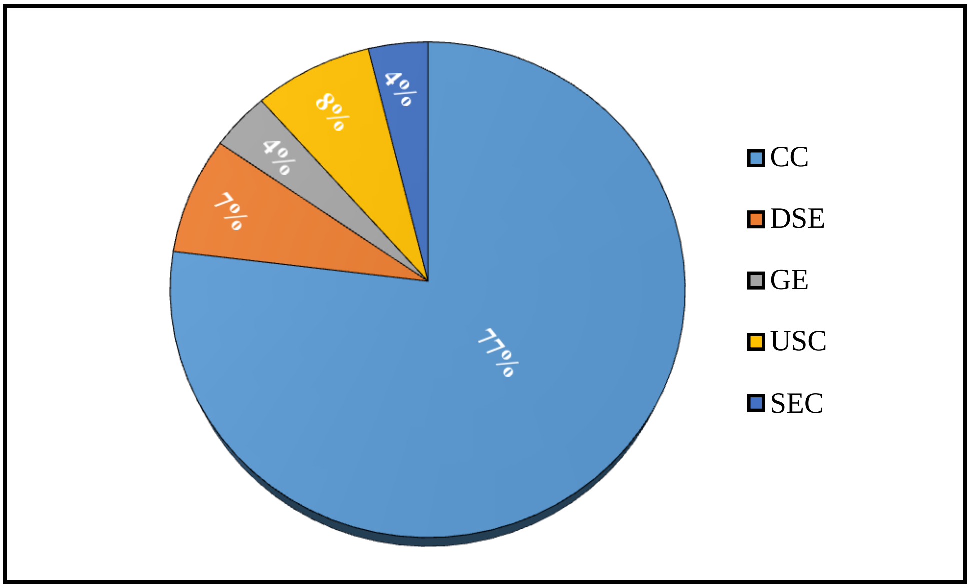
Total Credit

Year	Semester	hrs./Week	Credit
1st	1st	31	27
	2nd	31	27
2nd	3rd	31	27
	4th	43	23
Total			104

Category Codification with Credit Break up

Definition of Category	Code	No	Credit
Core Course	CC		80
Discipline Specific Elective	DSE		8
General Elective	GE		4
University specified course	USC		8
Skill Enhancement Course	SEC		4
Total			**104**

Category wise Credit Distribution



FIRST YEAR
SEMESTER – I

Mandatory Induction Program – Duration 3 weeks

- Physical Activity
- Creative Arts
- Universal Human Values
- Literary
- Proficiency Modules
- Lectures by Eminent

Category	Course name	Code	Credit	Teaching Scheme		
				L	T	P
CC – 1	Coordination Chemistry I & II, Molecular Cluster & Bioinorganic Chemistry I & II		4	4	0	0
CC – 2	Stereochemistry and Study of Reactive Intermediates		4	4	0	0
CC – 3	Advanced Spectroscopy I & Methods of Organic Synthesis		4	4	0	0
CC – 4	Statistical Mechanics, Thermodynamics and Quantum Chemistry		4	4	0	0
CC – 5	M.Sc. Chemistry Practical – I & II (Organic & Inorganic)		4	0	0	8
GE - 1	Generic Elective		4	4	0	0
USC – 1	Foreign language – I		2	2	0	0
SEC – 1	Mentored Seminar – I		1	1	0	0
Total Credit = 27 (CC: 20; GE: 04; USC:02; SEC: 01)				**Teaching Hour = 31 (hrs/week)**		

FIRST YEAR
SEMESTER – II

Category	Course name	Code	Credit	Teaching Scheme		
				L	T	P
CC – 6	Group Theory; Supramolecular Chemistry and Chemistry of d-and f-block Elements		4	4	0	0
CC – 7	Magnetochemistry I & II and Advanced Spectroscopy		4	4	0	0
CC – 8	Photochemistry & Special Name Reactions & Pericyclic Reactions		4	4	0	0
CC – 9	Advanced Spectroscopy-II and Diffraction Techniques		4	4	0	0
CC – 10	M.Sc. Chemistry Practical – III & IV (Physical & Organic)		4	0	0	8
DSE – 1	Biophysical Chemistry and Instrumentation		4	4	0	0
USC – 2	Foreign language – II		2	2	0	0
SEC – 2	Mentored Seminar – II		1	1	0	0
Total Credit = 27 (CC: 20; DSE: 04; USC:02; SEC: 01)				**Teaching Hour = 31(hrs/week)**		

SECOND YEAR
SEMESTER – III

Category	Course name	Code	Credit	Teaching Scheme		
				L	T	P
CC – 11	Homogeneous Catalysis and Catalysis in Industry, Chemistry of Cement and Ceramics, Electroanalytical techniques		4	4	0	0
CC – 12	Chemistry of biomolecules and Natural Products		4	4	0	0
CC – 13	Chemical Kinetics, Surface Chemistry and Macromolecules		4	4	0	0
CC – 14	Polymer Chemistry and Nanotechnology		4	4	0	0
CC – 15	M.Sc. Chemistry Practical – V & VI (Inorganic & Physical)		4	0	0	8
DSE – 2	Pharmaceutical Science and Drug Delivery		4	4	0	0
USC – 3	Foreign language – III		2	2	0	0
SEC – 3	Mentored Seminar – III		1	1	0	0
Total Credit = 27 (CC: 20; DSE: 04; USC:02; SEC: 01)				**Teaching Hour = 31 (hrs/week)**		

SECOND YEAR
SEMESTER – IV

Category	Course name	Code	Credit	Teaching Scheme		
				L	T	P
CC – 16	Chemistry Master Project / Dissertation	1080023518	20	0	0	40
USC – 4	Foreign language – IV		2	2	0	0
SEC – 4	Chemistry Master Seminar	5080023504	1	1	0	0
Total Credit = 23				**Teaching Hour = 43 (hrs/week)**		

Detail Curriculum for

M.Sc. CHEMISTRY

Organic Chemistry

First Year

Semester-I

CC-2: Stereochemistry and Study of Reactive Intermediates

(Credits: 4; Lecture – 04, Tutorial – 00, Practical - 00)

Component: Theory **CC-2** **Credits: 4**

(60 Lectures)

Unit 1: Organic Stereochemistry: **26 L**

Molecular symmetry and chirality. Symmetry operations and symmetry elements, point group classification and symmetry number.

Stereoisomerism. Classification, racemic modification, molecules with one, two or more chiral centres; configuration nomenclature D L R S and E Z nomenclature. Axial and planar chirality. Stereochemistry and configurations of allenes, spiranes, alkylidine cycloalkanes, biphenyls (atropisomerism), bridged biphenyls. Topicity and prostereoisomerism.

Cyclostereoisomerism. Configurations, conformations and stability of cyclohexanes (mono-, di-, trisubstituted), cyclohexanes, cyclohexanones, halocyclohexanones, decalins.

Asymmetry induction. Cram's Prelog's and Horeau's rules, Dynamic stereochemistry (acyclic and cyclic) Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle.

Unit 2: Study of Reactive Intermediates: **26 L**

A review of types of reactions of Organic Compounds.

Types of Reactive Intermediates and electron delocalization effects on stability of them.

Carbocations: Classical and nonclassical neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridgehead carbocations.

Carboanions: Generation, Structure and stability, and their general reactions.

Carbon-Carbon Bond Formation with Carbanions

Acidity of α-Hydrogen, α-Alkylations of Ketones and related compounds, S_N2 type reactions with carbanions, Nucleophilic addition of carbanions to carbon, Nucleophilic conjugated addition of carbanions, Stabilized carbanions or enolates from active methylene compounds, EAA synthesis, Malonic ester synthesis (DEM), keto-enol tautomerism.

Radicals: Generation, Structure, stability and reactions, cage effects, radical-cations & radical-anions, Reactions of free radicals.

Benzynes: Formation and Structure, different reactions of benzynes.

Carbenes: Formation and Structure, reactions involving carbenes.

Nitrenes: Generation, structure and reaction of nitrenes.

HSAB principle and its applications.

Structural Effects on Reactivity: Linear free energy relationships (LFER), the Hammett equation, substituent constants, theories of substituent effects, interpretation of σ-values, reaction constant ρ, deviations from Hammett equation, dual - parameter correlations, inductive substituent constant, the Taft equation.

Unit 3: Organometallic Compounds: **8 L**

Organolithium compounds, Organomagnesium compounds, Organoboron compounds, Suzuki coupling, Heck coupling, Sonogashira, Stille coupling, Kumada coupling, Organocopper compounds (Gillmann reagent), Organosilicon compounds, Organozinc compounds, Reformatsky reaction, Simmon-Smith cyclo propanation of alkenes.

References

1. Finar I L & Finar A L Organic Chemistry Vol.2 Addison-Wesley (1998)
2. Finar I L Organic Chemistry Vol.1 Longman (1998)
3. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee Organic Chemistry Seventh Edition, by Pearson (2018)
4. Leroy G. Wade, Junior, Organic Chemistry, 8th Edition by Pearson.

5. Eliel E L Stereochemistry of Carbon Compounds by Textbook Publishers (2003)

Course Outcomes:

CO1: Learn about molecular symmetry & chirality: axial & planar chirality as well as helicity.

CO2: Understand the details of conformational analysis of different cyclic and acyclic molecules including cyclohexanes, decalins etc.

CO3: Understand dynamic stereochemistry (acyclic and cyclic) and qualitative correlation between conformation and reactivity.

CO4: Learn about preparation and stability of different types of Reactive Intermediates like carbocation (both classical and non-classical), carbanion, nitrenes, carbenes, benzynes and their involvement in different types of organic chemical reactions.

CO5: Understand the structural effects on reactivity of organic substrates based on LFER, Hammett and Taft equations.

CO6: Learn about the chemistry of Organometallic compounds and different types of transition metal catalysed cross-coupling reactions.

CC-3: Advanced Spectroscopy I &
Methods of Organic Synthesis

(Credits: 4; Lecture – 04, Tutorial – 00, Practical - 00)

Component: Theory **CC3** **Credits: 4**

(60 Lectures)

Unit 1: Advanced Spectroscopy I **36 L**

1. Proton NMR Spectroscopy

Principle, instrumentation and different techniques of NMR spectroscopy, Fourier Transform NMR Spectroscopy, Characteristics values of Chemical Shifts, Spin-Spin splitting, Coupling constants, Origin of spin-spin splitting, Pascal's Triangle, One-Bond/Two-Bond/Three-Bond/Long-Range Coupling. Effect of solvent and hydrogen bonding on chemical shift.

2. Carbon-13 NMR Spectroscopy

Introduction to 13C-NMR spectroscopy, Spin-Spin splitting, DEPT 13 C NMR, application of NMR spectroscopy and other spectroscopically techniques to simple structural and mechanistic problems. Rules for carbon-13 calculations, principles of decoupling, Nuclear Overhauser effect. 2D NMR: NOESY, COSY, HSQC. Nuclear Magnetic Resonance Imaging.

3. Mass Spectroscopy

Basic Principles of EI: Electron Impact Ionization, Basic Principles of HRMS, Fragmentation Pattern of Small molecules in Mass Spectrometry, Problems incorporating Spectroscopic data, Fragmentation giving resonance stabilized data. Molecular ion, metastable ion, isotope peak, McLafferty rearrangement, nitrogen rule.

Unit 2: Methods of Organic Synthesis **24 L**

1. Heterocyclic Chemistry:

Synthesis, reactions and mechanisms of heter-aromatics containing more than one hetero atom: Imidazole, Pyrazole, oxazole, thiazole, isooxazole, isothiazole, pyrazines.

2. The Disconnection approaches:

Basic principles, guidelines for disconnection with special emphasis on chemo-selective, regioselective, stereoselective and stereospecific reactions, functional group inter conversion, synthon and reagent, synthetic equivalent, illogical electrophile and illogical nucleophile, Umpolong synthesis. designing synthesis of some target molecules with proper retrosynthetic analysis: Menthol, Penicillin V, Reserpine etc.

References

1. Finar I L & Finar A L Organic Chemistry Vol.2 Addison-Wesley (1998)
2. Finar I L Organic Chemistry Vol.1 Longman (1998)
3. Banwell, C.N.; McCash, E.M. Fundamentals of Molecular Spectroscopy, 4th Edition, India Edition, Tata McGraw-Hill, India.
4. Carruthers, W; Coldham, I. Modern Methods of Organic Synthesis, 4th Edition, Cambridge Publication.
5. Clayden J.; Greeves N.; Warren S. Organic Chemistry, 2nd Edition, Pearson Education India.
6. Kar, R. K. Fundamentals of Organic Synthesis: the Retrosynthetic Analysis, Volume 2, NCBA Publication.
7. Kalsi, P.S. Spectroscopy of Organic Compounds, Seventh Edition, New Age Publications, India.
8. Jag Mohan, Organic Spectroscopy: Principles & Applications, 2nd Edition, Narosa Publication, India.

Course Outcomes:

CO1: Learn about principle and instrumentation of ^{1}H NMR spectroscopy. Also acquire knowledge about chemical shifts, spin-spin splitting and coupling constants.

CO2: Learn about ^{13}C NMR spectroscopy, NOE and 2D NMR including NOESY and COSY.

CO3: Learn about Mass spectrometry in details including fragmentation giving resonance-stabilized data, Molecular ion and isotope peak and McLafferty rearrangement.

CO4: Develop skills to solve problems related to Spectroscopic data.

CO5: Learn about the chemistry of some important Heterocyclic compounds and their application in organic synthesis.

CO6: Understand retrosynthesis of organic molecules. Also gain knowledge of total synthesis of important complex organic molecules.

CC-5: MSc Practical I: Organic Chemistry

(Credits: 2; Lecture – 00, Tutorial – 00, Practical - 02)

(60 Lectures)

(*Experiments will be conducted based on availability of apparatus and reagents*)

List of practicals:

1. Acetylation of Aniline
2. O-Acylation of α-naphthol and phenol
3. Amino acid separation by TLC
4. Benzoic acid preparation,
5. Recrystallisation of benzoic acid and Melting Point determination
6. Synthesis of imine from carbonyls and amines.
7. Preparation of Benzalacetophenone from Benzaldehyde and Acetophenone and its chromatographic separation.

Text & Reference books:

1. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, *5th Ed.*, Pearson (2012)
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
3. Nad, A.K.; Mahapatra B.; Ghosal A. *Advanced Course In Practical Chemistry*, New Central Book Agency Ltd.
4. Subhash C Das, *Advanced Practical Chemistry*, (2012)

Course Outcomes:

CO1: Perform the acylation of anilines and phenols.

CO2: Identification and separation of different amino acids using TLC technique.

CO3: Preparation and recrystallisation of benzoic acid and determination of its melting point.

<u>SEMESTER-II</u>

CC-8: Organic Chemistry III:
Photochemistry & Special Name Reactions & Pericyclic Reactions

(Credits: 4; Lecture – 04, Tutorial – 00, Practical - 00)

Component: Theory **Organic Chemistry III** **Credits: 4**

(60 Lectures)

Unit 1: Photochemistry 16 L

Basic principles: Different types of electronic transitions in organic molecules: Jablonski diagram, direct and sensitized reactions;

Photochemistry of alkenes: cis-trans isomerization; Zimmermann reaction.

Photochemistry of Carbonyl compounds: Patterno-Buchi reaction, Norish Type I and Norish type II reaction, photo-reduction of ketone; photolabile protecting group.

Photorearrangements: Di-π methane rearrangement;

Photolysis of diazo compounds (generation of Carbenes);

Photochemistry of vision.

Unit 2: Special Name Reactions 16 L

Shapiro reaction, Mitsonobu reaction, Hofmann-Loffler-Freytag reaction, Barton reaction, Mannich reaction, Michael addition, Robinson annulation, Barton decarboxylation and deoxygenation reaction, Sharpless asymmetric epoxidation, Tandem cycloaddition reaction.

Peterson's Synthesis, Woodward and Prevost hydroxylation, Nef reaction, Ene reaction, McMurry coupling, Stile coupling, Wolff aromatization, Yamaguchi esterification, Brook, Neber, Stieglitz and Tiemann rearrangement, Corey-Fuchs reaction, Corey-Bakshi-Shibata reaction, Corey-Winter reaction, Wharton olefination, Fukuyama reaction, Fleming-Kumada oxidation, Buchner ring expansion, Takai olefination.

Unit 3: Olefin Metathesis **4 L**

Grubbs Reaction, Schrock Carbene, Fischer Carbene, Peterson, Julia Olefination.

Unit 4: Pericyclic Reactions **24 L**

Diels Alder cycloaddition reaction:

Dienophile, Diene, Regiochemistry, Stereochemistry, Intramolecular DA reactions, Retro DA reaction, Assymatric DA reactions.

[2+2] cycloaddition reaction

1,3 dipolar cycloaddition reaction

[3,3] sigmatropic rearrangement:

Cope rearrangement, Claisen rearrangement,

[2,3] sigmatropic rearrangement: Wittig rearrangement

Electrocyclic reactions

References:

1. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee Organic Chemistry Seventh Edition, by Pearson (2018)
2. Leroy G. Wade, Junior, Organic Chemistry, 8th Edition by Pearson.
3. .
4. Finar I L & Finar A L *Organic Chemistry Vol.2* Addison-Wesley (1998)
5. Finar I L *Organic Chemistry Vol.1* Longman (1998)
6. William Carruthers and Iain Coldham *Modern Methods of Organic Synthesis* Fourth Edition (2016) Cambridge.
7. Advanced Organic Chemistry - J. March.
8. Mechanism and Structure in Organic Chemistry - E. S. Gould.
9. Organic Photochemistry - J. W. Coxon & B. Halton.
10. Arun Bahl, B. S. Bahl, Advanced Organic Chemistry, 5th Edition by S. Chand
11. Elements of Organic Photochemistry - D. O. Cowan & K. L. Drisco.
12. Spectrometric Identification of Organic Compounds – R. M. Silverstein & F. O. Webster; 6th edition
13. Organic Spectroscopy – W. Kemp, 3rd Edn.

Course Outcomes:

CO1: Learn about different types of electronic transitions occurring in organic molecules, Jablonski diagram, direct and sensitized reactions. Also learn about photo induced reactions of different classes of organic compounds.

CO2: Learn about Photochemistry of Carbonyl compounds namely Patterno-Buchi reaction, Norrish Type I and Norrish type II reaction and photo-reduction of ketone.

CO3: Acquire knowledge about different organic name reactions with their mechanisms including Shapiro reaction, Mitsonobu reaction, Hofmann-Loffler-Freytag reaction, Barton reaction, Mannich reaction etc.

CO4: Learn critical olefin metathesis reaction namely Grubbs Reaction, Schrock Carbene, Fischer Carbene, Peterson and Julia Olefination.

CO5: Understand pericyclic reactions in the light of FMO approach and its application in Electrocyclic and cycloaddition reaction.

CO6: Learn about different sigmatropic reactions namely [3,3] sigmatropic rearrangement (Claisen and Cope), [2,3] sigmatropic rearrangement and Wittig rearrangement.

CC-10: MSc Practical IV: Organic Chemistry

(Credits: 2; Lecture – 00, Tutorial – 00, Practical - 02)

(60 Lectures)

(*Experiments will be conducted based on availability of apparatus and reagents*)

List of practical:

1. (a) Preparation of dibenzal acetone from acetone and benzaldehyde via Aldol condensation.

   (b) Purification and characterization of the product (by re-crystallization, TLC, determination of R_f value).
2. (a) Preparation of β-nitro styrene from benzaldehyde and nitromethane using Henry reaction.

   (b) Purification and characterization of the product (by re-crystallization, TLC, determination of R_f value).
3. (a) Ester preparation: Ethyl benzoate from Benzoic acid.

   (b) Purification and characterization of the product (by re-crystallization, TLC, determination of R_f value).
4. (a) Bromination: 2,4,6-Tribromophenol from phenol.

   (b) Purification and characterization of the product (by re-crystallization, TLC, determination of R_f value).
5. (a) Preparation from Picrate derivative (Charge Transfer Complex) from Picric acid and Acenaphthene.

   (b) Purification and characterization of the product (by re-crystallization, TLC, determination of R_f value).
6. (a) Preparation of Anthranilic Acid from Pthalimide.

   (b) Purification and characterization of the product (by re-crystallization, TLC, determination of R_f value).

Text & Reference books:

1. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, *5th Ed.*, Pearson (2012)
2. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)

3. Nad, A.K.; Mahapatra B.; Ghosal A. *Advanced Course In Practical Chemistry*, New Central Book Agency Ltd.
4. Subhash C Das, *Advanced Practical Chemistry*, (2012).

Course Outcomes:

CO1: Learn the synthetic methods for the preparation of dibenzal acetone and its purification and recrystallization.

CO2: Learn the synthetic methods for the preparation of β-nitro styrene from benzaldehyde and nitromethane using Henry reaction, its purification, recrystallization and characterization.

CO3: Learn the synthetic methods for the preparation of Ethyl benzoate from Benzoic acid and recrystallisation and characterization of the product.

Second Year

Semester – III

CC – 12: Chemistry of biomolecules and Natural Products

(Credits: 4; Lecture – 04, Tutorial – 00, Practical - 00)

Component: Theory **CC-12** **Credits: 4**

(60 Lectures)

<u>Unit 1: Nucleic acids</u> **14 L**

Introduction, Ribonucleosides and Ribonucleotides, Purine and Pyrimidine.

The structure of Ribonucleic Acid, Deoxyribose and Deoxyribonucleic acid, Base Pairing, The Double Helix of DNA.

Additional Functions of Nucleotides, Chemistry and heredity, The genetic code and control of Protein biosynthesis, Polymerase chain reaction.

Various forms of DNA (a, b, c, z) and RNA (m, r t).

<u>Unit 2: Amino Acids & Proteins</u> **14 L**

Introduction, Structure and stereochemistry of α–Amino Acids, Acid-Base properties of Amino Acids, Isoelectric points and Electrophoresis, Synthesis of Amino Acids, Resolution of Amino Acids, Reactions of Amino Acids.

Classification of Proteins, Levels of Protein Structure, Protein Denaturation.

Natural and synthetic amino acids, Canonical and non-canonical amino acids, Different synthetic strategy of peptides, Structure and function of protein and chemistry behind protein biosynthesis. Ramachandran plot, denaturation of proteins, factors affecting denaturation, protein folding. Unnatural Amino Acid.

<u>Unit 3: Carbohydrates</u> **14 L**

Introduction, Classification of Carbohydrates, Monosaccharides, Erythro and Threo Diastereomers, Epimers, Cyclic structures of Monosaccharides, Anomers of Monosaccharides: Mutarotation.

Reactions of Monosaccharides: side reactions in Base, Reduction of Monosaccharides, Chain shortening: The Ruff degradation, Chain lengthening: The Kiliani-Fischer Synthesis. Disaccharidses and Polysaccharides.

Unit 4: Chemistry of Natural Products **18 L**

Steroids: Cholesterol, Sex Hormones, Adrenal Steroids, Anabolic Steroids.

Alkaloids: Occurrence and Isolation, General properties, Classification, Determination of Structure, Conine, Quinine, Nicotine, Atropine.

Terpenes (Terpenoids): Isoprene Rule (C5 Rule), Myrcene, Citral, Geraniol, Nerol.

Vitamins: Classification of Vitamins: Vitamin A, Vitamin B (complex), Vitamin C, Vitamin D, Mechanisms of Actions.

References:

1. R. T. Morrison, R. N. Boyd, S. K. Bhattacharjee, Organic Chemistry Seventh Edition, by Pearson (2018)
2. Leroy G. Wade, Junior, Organic Chemistry, 8th Edition by Pearson.
3. Finar I L & Finar A L *Organic Chemistry Vol.2* Addison-Wesley (1998)
4. Finar I L *Organic Chemistry Vol.1* Longman (1998)
5. Arun Bahl, B. S. Bahl, Advanced Organic Chemistry, 5th Edition by S. Chand

Course Outcomes:

CO1: Learn about Purine and Pyrimidine bases, Ribonucleosides and Ribonucleotides and Structure of Ribonucleic Acid.

CO2: Learn about Structure of Deoxyribose and Deoxyribonucleic acid and Double Helix of DNA.

CO3: Learn about the stereochemistry of α-Amino Acids, their properties, Synthesis, Resolution and Reactions of Amino Acids.

CO4: Learn about the classification, structure and denaturation of protein. Also acquire knowledge about protein biosynthesis and polymerase chain reaction.

CO5: Learn about the detailed structure, stereochemical aspects and reactions of carbohydrates.

CO6: Gain knowledge about the structure elucidation, properties and reactions of Steroids, Alkaloids and Terpenoids and Vitamins.

Semester – IV

CC – 16: Chemistry Master Project & Dissertation

(Credits: 20; Lecture – 00, Tutorial – 00, Practical - 40)

Chemistry Master Project & Dissertation **Credit: 20**

A research project work should be done individually under the guidance of one (or more) faculty of Chemistry department at SNU or anywhere else on any topic related to the subject & can be recorded as dissertation & also be presented by the candidate in front of external and internal examiners in a seminar presentation. Project may be divided into two parts: the first part (of credit 04) would be carried out after second semester for one month. The second part (of credit 04) would be carried out during fourth semester.

TWO YEAR SYLLABUS

OF

Master of Science in

CHEMISTRY

Vice-Chancellor,

Sister Nivedita University

Subject Expert

Raj K Datta

Chief General Manager - Product Development, Technical Support & QA

Haldia Petrochemicals Limited

Industry Expert

Head of the Department,
Chemistry, SNU

Detail Curriculum for

M.Sc. CHEMISTRY

(Inorganic Chemistry)

First Year

Semester-I

MS-CC 1: Inorganic Chemistry I:

Coordination Chemistry I & II, Molecular Clusters and Bioinorganic Chemistry I & II

(Credits: 6; Lecture – 04, Tutorial – 00, Practical - 02)

Component: Theory **Inorganic Chemistry I** **Credits: 4**

(40 Lectures)

Unit 1: Coordination Chemistry I: **7 Lectures**

Crystal Field Theory: Spitting of d orbitals in crystal fields of different symmetry for similar and dissimilar ligands (Octahedral, tetrahedral, Linear, trigonal planar, trigonal bipyramidal, square pyramid), crystal field stabilization energies (CFSE), spectrochemical series, octahedral site preference energy (OSPE) and their applications. Tetragonal distortion (John-Teller effect).

Unit 2: Coordination Chemistry II: **8 Lectures**

Thermodynamic aspects of crystal field splitting (variation of ionic radii, lattice energy, hydration enthalpy and stability constants of complexes –Irving Williams order). Kinetic aspects of crystal field stabilization: crystal field activation energy, labile and inert complexes. Spin and orbital moments, spin-orbit coupling, quenching of orbital moment, spin only formula, temperature dependence of magnetic moment, Super exchange Phenomena, Diamagnetic Corrections. Dependence of Orbital contribution on the nature of the electronic ground state. Microstates, terms and energy levels for $d^1 – d^9$ ions in cubic and square fields - selection rules - band intensities and band widths - Orgel and Tanabe-Sugano diagrams.

Unit 3: Molecular Clusters: **10 Lectures**

Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the *closo*-, *nido*-, *arachno*-borane structural paradigm**,** styx No. of neutral and boron hydrides, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity. Transition-metal clusters: Capping rules, metal-ligand complexes vs heteronuclear cluster. Main-group-Transition-metal clusters: Isolobal analogs of p-block and d-block clusters, limitations and exceptions. Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters. Metal-carbonyl clusters, structures, capping and electron counting. Molecular clusters in catalysis, clusters to materials, boron-carbides and metal-borides. Illustrative examples from recent literature.

Unit 4: Bioinorganic Chemistry –I : **7 Lectures**

Introduction: A review of Metals in Biology, Medicine and Biogeochemical Cycles; Introduction to Biochemistry & Metal Ions and Proteins: Binding, Stability, and folding, Special Cofactors.

Unit 5: Bioinorganic Chemistry –II: **8 Lectures**

Metal clusters Metal Ion Transport and Storage; Heme Fe – O2 Carriers (Myoglobin, Hemoglobin) O2 Activation (Hr, Hc, P450), Non-Heme Fe – O2 Activation; O2 Reduction – Cytochrome c Oxidase; O2 Evolution – Photosystem II, O2 toxicity – SOD, Catalase, Peroxidase, Metalloenzymes with Radical Intermediates (Cobalamins, Fe-S clusters and Sadenosyl methionine).

References Books

1. Atwood J L & Steed J W Supramolecular Chemistry A Concise Introduction John Wiley & Sons (2000)
2. Adamson A.W. & Fleischauer, P.D. (Eds) Concepts of Inorganic Photochemistry Wiley

New York (1975)

3. Inczedy J Analytical applications of complex equilibria Halsted Press, New York, NY (1976)
4. Ringbom A. Complexation in Analytical Chemistry Wiley, New York (1963)
5. Beck M T Chemistry of Complex Equilibria van Nostrand Reinold New York (1970)

Course Outcomes:

CO1: Illustrate Crystal Field Theory and thermodynamic aspects of crystal field splitting.

CO2: Demonstrate super exchange phenomena, diamagnetic corrections, dependence of orbital contribution on the nature of the electronic ground state.

CO3: Expertise on main-group clusters and their structural aspects and electronic properties

CO4: To **discuss** and list the role of alkaline earth metals in biological systems.

CO5: To **explain** and examine the role of Iron, copper and molybdenum proteins with reference to their oxygenation and oxidase activity in biological systems.

CO6: To **describe** and **show** the different roles of metalloenzymes in biological systems

CC-5: MSc Practical II: Inorganic Chemistry

(Credits: 4; Lecture – 00, Tutorial – 00, Practical - 04)

(*Experiments will be conducted based on availability of apparatus and reagents*)

Inorganic Chemistry **Credits: 2**

1. Synthesis and characterization of inorganic and coordination compounds. Characterization techniques to be used for each experiments (*wherever applicable*) are XRD, UV-vis,,FT-IR, TGA/DTA, Surface Area analysis (BET), Magnetic susceptibility measurements, Cyclic Voltammetry, ICP-MS and AAS
2. Determination of phosphoric acid in soft drinks
3. Estimation of Alkali content in Antacid Tablet
4. Estimation of calcium in milk powder by complexometry
5. Synthesis of ferrocene derivative and measurement of redox potential using cyclic voltammetric methods.

Course Outcomes:

CO1: To analyze complex material by various instrumental methods

CO2: To develop hands on experience on making various inorganic compounds by employing a variety of synthetic strategies and their characterization will be aimed

CO3: To impart advanced knowledge on the quantitative analysis of metals as their complexes.

SEMESTER-II

CC-6: Inorganic Chemistry II:

Group Theory; Supramolecular Chemistry and Chemistry of d-and f-block Elements

(Credits: 6; Lecture – 04, Tutorial – 00, Practical - 02)

Component: Theory **Inorganic Chemistry II** **Credits: 4**

(40 Lectures)

Unit 1: Group Theory **10 Lectures**

Definition of group, symmetry, point groups, representation of group, Abelian group, Group multiplication table, Groups, sub-groups and classes, Symmetry operations and symmetry elements, Point group, classification and symmetry number, Selection Rules, Schoenflies symbols. Great Orthogonality Theorem, irreducible representation, character table, Point group symmetry

Unit 2: Applications of Group Theory **10 Lectures**

Optical activity, dipole moment, vibrational spectroscopy and bonding. Crystal field splitting of free ion terms in weak and strong crystal fields (Oh and Td), Walsh diagram & its application towards molecular geometry.

Unit 3: Supramolecular Chemistry **15 Lectures**

Introduction to supramolecular chemistry (concepts and definitions), Nature and types of supramolecular interactions (Hydrogen bonding, van der Waal interactions, π-stacking, C-H….π interactions, hydrophobic effects, solvation, etc.), Concepts and terminology of supramolecular chemistry—Cooperativity, chelate effect, macrocyclic effect, host-guest complementarity, Preorganisation and complementarity.

Molecular recognition- Principle of molecular recognition, Different types of receptors with special reference of Crown ethers, Podands, cryptands, spherands; Synthesis of cryptands-template effect.

Anion recognition: challenges in anion receptor chemistry, host design for anion; anion coordination chemistry. Self-assembly- formation and examples. Application of supramolecular chemistry.

Unit 4: Chemistry of d--block elements (Transition Elements) **8 Lectures**

Electronic configuration, oxidation states; aqueous, redox and complex chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d,4d, and 5d elements with references to Ti-Zr- Hf , Cr- Mo- W, Mn-Tc-Re and Pt group metals. Occurrence and isolation in respect of Mo, W, Re, Pt. Synthesis, properties, reactions, structure and bonding as applicable in respect of: Mo-blue, W-blue, Pt-blue, W-bronze, Ru-red, Creutz- Traube complexes, Vaska`s complexes.

Unit 5: Chemistry of f-block elements (Lanthanide and Actinide Elements) **7 Lectures**

Lanthanide and Actinide Elements: Nuclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-, redox- and complex-chemistry; electronic spectra and magnetic properties. Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (examples).

Reference Books:

1. J. D. Lee, Concise Inorganic Chemistry, Chapman and Hall, London, 1991.
2. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Edn, Pergamon, New York, 1997.
3. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons, Inc, New York, 1999.
4. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.
5. G. L. Miessler and D. A. Tarr, Inorganic Chemistry, 3rd Edn, Pearson, New Delhi, 2009.
6. C. E. Housecroft, Cluster Molecules of the p-Block Elements, Oxford University Press, Cambridge, 1994.
7. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Shriver & Atkins Inorganic Chemistry, 4th Edn, Oxford, 2006.

Course Outcomes:

CO1: To **discuss** group theory to recognize and assign symmetry characteristics to molecules.

CO2: How to **apply** the knowledge of fundamental chemistry to characterize new molecules.

CO3: To **discuss** and **describe** the applications of widely used experimental technique of Supramolecular Chemistry.

CO4: Develop knowledges on main-group-transition-metal clusters: isolobal analogs of p-block and d-block cluster

CO5: Illustration of salient features and characteristic properties of d-and f-block elements.

CO6: Develop knowledge on magnetic, optical and useful properties of d- and f-block elements.

CC-7: Inorganic Chemistry III:

Magnetochemistry I & II and Advanced Spectroscopy

(Credits: 6; Lecture – 04, Tutorial – 00, Practical - 02)

Component: Theory **Inorganic Chemistry I** **Credits: 4**

(40 Lectures)

Unit 1: Magnetochemistry -I **8 L**

Magnetic properties of substances, orbital and spin angular momentum of electrons, paramagnetic moment and magnetic susceptibility. Paramagnetic and diamagnetic materials, ferromagnetism, ferrimagnetism, antiferromagnetism, magnetic permeability, magnetic susceptibility, magnetization, classical theory of diamagnetism and paramagnetism, diamagnetism and Pascal‟s constants, zero-field splitting, spin-orbit coupling. Determination of magnetic susceptibility by these methods: Gouy, Faraday, NMR method and SQUID.

Unit 2: Magnetochemistry –II **10 L**

Magnetic properties and temperature – The curie and Curie- Weiss law, derivation of Curie law. Microstates, hole formalism, multiplet, multiplet width, Lande interval rule, magnetic moments for different multiplet widths, crystal field diagram, quenching of orbital contribution, high spin/low spin equilibrium. Antiferromagnetic interactions in inorganic compounds: Mechanism like – direct interaction, superexchange interactions and elucidation with poly nuclear metal complexes as well as oxide and halide salts of transition metals.

Unit 3: Electron Spin Resonance Spectroscopy –I **8 L**

Basic principle, Hyperfine splittings (isotropic systems); the g-value and the factors affecting thereof; interactionsaffecting electron energies in paramagnetic complexes (Zero-field splitting and Kramers degeneracy).

Unit 4: Electron Spin Resonance Spectroscopy –II **6 L**

Anisotropic effects (the g-value and the hyperfine couplings); The EPR of triplet states; Structural applications to transition metal complexes.

Unit 5: Mössbauer Spectroscopy **8 L**

Basic principle, conditions for Mossbauer spectroscopy, Spectral parameters (Isomer shift, electric quadruple interactions, magnetic interactions), temperature dependent effects, structural deductions for iron and tin complexes.

Reference Books:

1. Atwood J L & Steed J W Supramolecular Chemistry A Concise Introduction John Wiley & Sons (2000)
2. Adamson A.W. & Fleischauer, P.D. (Eds) Concepts of Inorganic Photochemistry Wiley New York (1975)
3. Inczedy J Analytical applications of complex equilibria Halsted Press, New York, NY (1976)
4. Ringbom A. Complexation in Analytical Chemistry Wiley, New York (1963)
5. Beck M T Chemistry of Complex Equilibria van Nostrand Reinold New York (1970)

Course Outcomes:

CO1: Learn to predict and discuss the source of magnetic nature in any metal complex.

CO2: Develop knowledge about laws of magnetochemistry and antiferromagnetic interactions in inorganic compounds.

CO3: Learn to analyze magnetic susceptibility using various methods.

CO4: Analyze the magnetic properties of co-ordination compounds by applying the basic concepts of magneto-chemistry.

CO5: Develop expertise on the application of molecular spectroscopy in structure elucidation of compounds.

CO6: Learn to correlate electronic features to it property and applications in various field of science.

Second Year

Semester – III

CC-11: Inorganic Chemistry IV:

Homogeneous Catalysis and Catalysis in industry, Chemistry of Cements and Ceramics, Electroanalytical Techniques

(Credits: 6; Lecture – 04, Tutorial – 00, Practical - 02)

Component: Theory **Inorganic Chemistry III** **Credits: 4**

40 Lectures

Unit 1: Homogeneous Catalysis: ***8 Lectures***

Introduction to Catalysis, basic principles: Definition of activity, selectivity in catalysis; homogeneous vs. heterogeneous catalysis; importance of homogeneous catalysis in the synthesis of high value chemicals.

Characteristics of central metal ions and influence of attached ligands on catalytic activity; Important reaction types: Oxidative addition and reduction; elimination, insertion (migratory) reactions, β-hydride elimination.

Polymerization: Catalytic cycle for alkene polymerization; Metallocene catalysts, structure, special features and advantages of metallocene catalysts; mechanism of polymerization and stereocontrol by metallocene catalysts.

Unit 2: Catalysis in industry ***8 Lectures***

Industrial applications of organotransition metal compounds; Important catalytic reactions: Hydrogenation, Wacker process, Ziegler-Natta catalysis; Metal carbonyls compounds; Organometallic reagents in organic synthesis: Principle, preparation and applications of Li, Mg, Hg, Zn, Ni, Pd, Fe, Co and boron compounds in organic synthesis.

Unit 3: Chemistry of Cement: **8 Lectures**

Indian Cement Industry, Cement Manufacturing Process, Cement Raw Materials, Corrective Materials/ Additives. Raw Mix Proportioning, Raw Mix Design, 89 Modulii Values and their effects. Burnability, Absorption and effect of Coal Ash. Chemical and Phase Composition of Clinker, Bogue Calculation, Clinker Reaction during Clinkerization, Fuels, Mineralisers and Fluxes. Hydration of Cement, Setting, Hardening and Strength gain, Role of various Clinker Phases. Use of Waste Materials – Fly ash and Slag etc., Pozzolanic Reaction, Hydration of Slag. Types of Cement, BIS specifications of various types of Cement

Unit 4: Chemistry of Ceramics — ***8 Lectures***

Ceramics: Historical development, Raw materials-their composition, occurrence, properties andclassification. Ceramic industries in India. Manufacture of white ware, drying and firing of ceramic products. Ceramic products whiteware porcelain, sanitaryware, glazes; advanced polymer based ceramic products, ceramic coating. Conventional Process – Dry and semi-dry pressing, Slip casting, Extrusion. Advanced Process – Cold Isostatic pressing & Hot Isostatic pressing, Injection moulding, Hot- pressing. Sintering: Solid-state sintering, Liquid Phase sintering and verification, Driving force Of Sintering, controlling factors for sintering of ceramic system.

Unit 5: Electroanalytical Techniques: — **8 Lectures**

Review of the basics of electrochemistry; Coulometry, coulometric titrations; potentiometry; descriptions of the double layer chronoamperometry, chronocoulometry, chronopotentiometry; electrolytic separations,polarography, voltammetry, and hydrodynamic electrochemical methods of analysis; voltammetry in quiescent solution, hydrodynamic voltammetry, impedance spectroscopy, chemically modified electrodes, Spectro-electrochemistry electrochemical imaging methods.

References:

1. J. D. Lee, Concise Inorganic Chemistry, Chapman and Hall, London, 1991.
2. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Edn, Pergamon, New York, 1997.
3. F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons, Inc, New York, 1999.

4. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.
5. Introduction of ceramics- W.D. Kingery, H. Kent Bowen, D.R. Uhlmann
6. Handbook of ceramic technology
7. Whiteware by Sudhir Sen
8. The Chemistry of Cement and Concrete, F. M. Lea
9. Cement Chemistry, H.F.W. Taylor
10. Homogeneous Catalysis: The Applications and Chemistry of Catalysis by Soluble Transition Metal Complexes, G.W. Parshall and S.D. Ittel, Wiley, New York 1992
11. 2. Applied Homogeneous Catalysis with Organometallic Compounds, Vols. 1 & 2, edited by B. Cornils and W.A. Herrmann, VCH, Weinheim, New York, 1996
12. 3. Homogeneous Catalysis: Mechanisms and Industrial Applications, S. Bhaduri and D. Mukesh, Wiley, New York, 2000
13. 4. Homogeneous Catalysis: Understanding the Art, P.W.N.M. van Leeuwen, Kluwer Academic Publishers, 2003

Course Outcomes:

CO1: Illustrate the basic terms related to Catalysis and demonstrate the quantitative and qualitative idea about heterogeneous and homogeneous catalysis, adsorption and reaction kinetics.

CO2: State about commodity and general-purpose thermoplastics (e.g. Polyethylene and other polymers) and elaborate the industrial manufacturing procedure of ceramics and their thermal properties as well as their uses

CO3: Demonstrate the industrial manufacturing procedure of cements and ceramics, and their chemical and thermal properties as well as their uses.

CO4: State various catalytic reactions, derive the rate equation for enzyme catalysis, and able to calculate the associated turnover numbers.

CO5: Illustrate how to construct the catalytic cycles and develop knowledge about various catalyst being used in different industries.

CO6: Demonstrate a theoretical as well as a practical introduction to principles and techniques of some electroanalytical techniques.

CC-15: MSc Practical V (Inorganic Chemistry)

(Credits: 4; Lecture – 00, Tutorial – 00, Practical - 04)

(*Experiments will be conducted based on availability of apparatus and reagents*)

Inorganic Chemistry **Credits: 2**

1. Preparation of nitro- and nitrito-pentamminecobalt (III) chloride and characterization using spectroscopic techniques
2. Preparation of Prussian blue and its character by UV-visible spectroscopy.
3. Preparation of ferrous ammonium sulphate, Mohr's salt $FeSO_4.(NH_4)_2SO_4.6H_2O$.
4. Preparation of *Schiff base* and metal complexes (*bi-metallic complexes*). Characterization techniques to be used for each experiments (*wherever applicable*) are XRD, UV-vis,,FT-IR, TGA/DTA, Surface Area analysis (BET), Magnetic susceptibility measurements, Cyclic Voltammetry, ICP-MS and AAS
5. Synthesis and characterization of ferrocene and acetylferrocene (Synthesis, purification using chromatography and characterization)

Course Outcomes:

CO1: Interpret and identify the fusion behavior of different inorganic compounds.

CO2: Develop skill on fusion test of different metal oxides.

CO3: Illustrate the analysis of unknown Inorganic samples.

CC – 16: Chemistry Master Project & Dissertation

(Credits: 20; Lecture – 00, Tutorial – 00, Practical - 40)

Chemistry Master Project & Dissertation **Credit: 20**

A research project work should be done individually under the guidance of one (or more) faculty of Chemistry department at SNU or anywhere else on any topic related to the subject & can be recorded as dissertation & also be presented by the candidate in front of external and internal examiners in a seminar presentation. Project may be divided into two parts: the first part (of credit 04) would be carried out after second semester for one month. The second part (of credit 04) would be carried out during fourth semester.

TWO YEAR SYLLABUS

OF

Master of Science in

CHEMISTRY

Vice-Chancellor,

Sister Nivedita University

Subject Expert

Raj K Datta

Chief General Manager - Product Development, Technical Support & QA

Haldia Petrochemicals Limited

Industry Expert

Head of the Department,
Chemistry, SNU

Detail Curriculum for

M.Sc. CHEMISTRY

Physical Chemistry

Semester-I

CC-4: Physical Chemistry I: Statistical Mechanics, Thermodynamics & Quantum Chemistry

(Credits: 4; Lecture – 04, Tutorial – 01, Practical - 00)

(60 Lectures)

Component: Theory **Physical Chemistry I** **Credits: 4**

Unit 1: Statistical Mechanics & Thermodynamics: **20 L**

Fundamentals and micro-canonial, canonical systems

Objective of statistical mechanics; Method of statistical mechanics, macrostates, microstates, probability, ensembles. Entropy and probability; Partition function; Equation of state; Energy fluctuation and C_v; Microcanonical and canonical distributions using Lagrange's undetermined multiplier; Entropy of an ideal gas mixture according to Classical Statistical Mechanics and Gibbs paradox.

Grand canonical system

Partition function; Equation of state; Fluctuation in the number of particles; PV = kTln Z relation.

Quantum statistical mechanics

Density matrix; Quantum Liouville theorem; Density matrices for microcanonical, canonical and grand canonicalsystems; Identical particles – BE and FD distributions. Ideal, Bose and Fermi gas: Equation of state; Bose condensation; Equation of state of ideal Fermi gas, Fermi gas at T = 0 K and above; Variation of Fermi energy with temperature and specific heat of free electron gas.

Unit 2: Quantum Chemistry **20 L**

Fundamentals of Quantum mechanics: Postulates of quantum mechanics, uncertainty principle, interpretation of wave function, properties of wave function, linear and hermitian operators, commutator, expectation energy and mean value theorem. Differential equations, partial differential equations, series solutions and special functions, linear vector spaces, transformation of coordinate matrix, representation of operators, eigen valueproblem, orthonormal sets, Fourier and Laplace transformation. Ladder operators. Rigid rotator and hydrogen atom. Complete solution. Radial distributions.Virial theorem.

Particle in a box and ring, quantum mechanical tunneling, quantum well, degeneracy of energy levels H-atom wave function, separation of translational and rotational parts of the Schrödinger equation, Quantum numbers and their significance, shapes of the orbitals, energy of H-atom orbitals.

Quantum mechanics and multielectronic atoms: Multielectronic atoms, wave functions, Self Consistent Field, Hartree-Fock method. Energy levels in multielectronic atoms and ground spectral states. Spectral states of polyelectronic atoms, LS and jj couplings, allowed microstates of d electrons and spectral states.

Approximate methods: Born-Oppenheimer approximation Variational treatment of hydrogen molecule ion. and their applications. First order time-independent perturbation theory for non-degenerate states. Variation theorem and variational methods, Time-dependant Schrodinger equation and its significance. Slater parameters and their relationship with energies of spectral states, Zeeman and Stark effects. Spectra of alkaline earth metal ions. Electrostatic concept of complex formation, effect of ligand field geometry on the energy of d-orbitals, factors affecting crystal field splitting, spectrochemical series, Jahn -Teller Theorem.

Unit 3: Group Theory **10 Lectures**

Quantum mechanics and group representation theory Reducible and irreducible representations, Character tables , Great Orthogonality theorem, Transition probability, Selection Rules, Projection operators, Direct product representation, Construction of SALC, Selection rules in spectroscopy, Study of normal modes, IR and Raman activity. Symmetry and chemical reactions; Woodward –Hoffmann Rule

Unit 4 : Lasers and their applications **10 L**

Two energy system and three energy systems, concept of lasers, few common lasers. Two level transition (absorption, induced and stimulated emission), Einstein model for two levels transition, Principle of Maser and Laser action. Basic element in laser (resonator, Gain medium, Pumping technique), Characteristics of laser radiation (coherence: temporal/spatial; polarization, monochromaticity, intensity), Single mode laser (solid/ gas laser: Ruby, Nd:YAG, Ar-ion, CO_2, Excimer etc.) tunable laser (Dye laser), Harmonic generation, Application of laser (chemical problem, medicinal and industrial).

References

1. Lowe, J P & Peterson K Quantum Chemistry Academic Press (2005)
2. Atkins, P. W., & Friedman, R. S. (2011). Molecular quantum mechanics. Oxford university press.
3. Levine, M., & Heath, A. (1991). Quantum chemistry.
4. McQuarrie, D. A., McQuarrie, D. A., McQuarrie, D. A., &McQuarrie, D. A. (1973). Statistical thermodynamics (pp. 304-305). New York: Harper & Row.
5. Reif, F. (2009). Fundamentals of statistical and thermal physics. Waveland Press.
6. Chemical Application of Group Theory – F.A.Cotton
7. Group theory and chemistry- D. M. Bishop

Course Outcomes (CO)

CO1: The student will have thorough knowledge on different classical and quantum mechanical distribution functions.

CO2: The student can explain the procedures for deriving the relation between thermodynamic parameters such as pressure, temperature, entropy and heat capacity from the distribution functions.

CO3: The student can explain phase transitions and magnetization in magnetic systems.

CO4: The student is able to understand molecular systems in the light of quantum theory.

CO5: The student will be able to understand how a molecule interacts with light.

CO6: The student will be able to predict properties of molecules through light matter interactions.

<u>Semester –II</u>

CC-9: Physical Chemistry II: Advanced Spectroscopy II & Diffraction Techniques

(Credits: 4; Lecture – 04, Tutorial – 00, Practical - 00)

Component: Theory **Physical Chemistry II** **Credits: 4**

(60 Lectures)

<u>Unit 1 : Rotational spectroscopy:</u> **10 L**

Electromagnetic radiation and its interaction with matter. Essential conditions, Rigid rotor model, diatomic and polyatomic molecules, linear, symmetric top and asymmetric top molecules; Energy values, quantization andselection rules, non-rigid rotor.

<u>Unit 2 : Vibrational spectroscopy:</u> **10 L**

Essential conditions, Models : Classical and Quantum oscillator; Selection rule, Anharmonicity, Hot bands, Vibration-Rotation spectra.

<u>Unit 3: Raman Spectroscopy:</u> **10L**

Essential conditions, Characteristics and Explanations; Drawbacks of classical theory; Vibrational and Rotational Raman.

<u>Unit 4: Electronic spectroscopy:</u> **20L**

Lambert Beer's Law: its uses, limitations, Optical transitions in a two- level system: Einstein's two level transition model; Transition moment; Selection rules with symmetry arguments; Different types of transitions (π–π^*, σ–π^*, n–π^* etc.); Solvent perturbation method; Weak and CT transition; Violation of selection rule: Vibronic and spin orbit coupling. Basic principle of luminescence; Photoluminescence: definition, types of luminescence; Fluorescence, phosphorescence, internal conversion, intersystem crossing anddelayed fluorescence; Jablonski diagram; FC principle; De-excitation processes, Parameters affecting de-excitation processes; Fluorescent Probes-extrinsic and intrinsic probes; Triplet– triplet transitions; Fluorescence

Lifetime measurement; Quantum yield; intramolecular charge transfer (ICT); Effects of molecular structure, environmental factors on fluorescence; Fluorescence quenching; Static and dynamic quenching; Stern–Volmer kinetics; Energy transfer; energy transfer to multiple acceptor; Photoinduced electron transfer; Excimer and exciplexformation; Photoinduced proton transfer; Fluorescence anisotropy; Basic knowledge on instrumentation of spectrophotometers

Unit 5: Spectroscopy and Quantum Mechanics **10 L**

Fundamentals of spectroscopy from Quantum and group theory. Selection rules, Transition moment integral and its significance. Deduction of Lambert Beers Law from quantum mechanics. Selection rule for vibrational spectra, anharmonic correction by perturbation - appearance of overtones, selection rule for rotational spectra, nuclear spin and energy levels, Stark effect, Raman scattering, selection rule for rotation-vibrational Raman effect. Nonlinear scattering- hyper – Raman, Stimulated and Resonance Raman spectra.

References:

1. Banwell and McCash, Fundamentals of Molecular Spectroscopy, 4th Edition, Tata McGraw Hill, 2010
2. Molecular Spectroscopy – I.N.Levine
3. Introduction to Molecular Spectroscopy by G. M. Barrow, McGraw Hill
4. N. J. Turro, Modern Molecular Photochemistry, University Science Books, 1991.
5. B. Valuer, Molecular Fluorescence, Wiley-VCH, 2002.
6. Modern Molecular Photochemistry by Nicholas J. Turro, University ScienceBooks, 1991.
7. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, Springer, 3rd Ed. 2006. Griffiths, D. J., &Schroeter, D. F. (2018). Introduction to quantum mechanics. CambridgeUniversity Press.

Course Outcomes:

CO1: The student will learn the interactions of electromagnetic radiation with matter – its concominent energy transfer between radiation and matter.

CO2: The student will learn the effect of rotation on the bond length and internal energy level of the molecule. This ultimately explains the appearance of spectral lines, gaps between the lines. Students will also learn to build idea on structure of (linear/ symmetric top) and bond length of molecules from Rotational Spectrum.

CO3: The students will learn about the modes of vibration of different molecules and will be able to calculate the energy values and frequency / wave number of transition among vibrational level. They will also learn the deviation from the classical system and appearance of different lines in the spectrum (IR) and will also learn to relate molecular structure / composition with IR lines.

CO4: The student will learn the essential features of scattering and will understand the difference between the spectroscopic methods based on scattering and absorption phenomena. They will understand different Raman active modes and the appearance of lines of different frequencies in Raman Spectroscopy. Relation of molecular structure with Raman lines will also be understood.

CO5: The student will learn in detail the electronic transitions due to absorption of electromagnetic radiation by matter and its consequences. Jablonsky diagram, mirror – image rule, FRET etc. phenomenon will be elaborately discussed.

CO6: Basic principles and instrumentation of monitoring diffraction pattern of solids will be studied and its applications in structure determination will be learnt.

DSE – 1: Biophysical Chemistry & Instrumentation

(Credits: 4; Lecture – 04, Tutorial – 00, Practical - 00)

Component: Theory **Credits: 4**

(60 Lectures)

Unit 1: Introduction to Biophysical Chemistry **2 L**

Central dogma of life and its molecular basis. Different macromolecules in biological systems: Proteins and peptides; Membranes; Lipids, Nucleic acids

Unit 2: Amino Acids **3 L**

α-amino acids – their structures, stereochemistry and optical activity; Properties of amino acids; peptide bonds; Polar and Non-polar amino acids; Essential and Non-essential amino acids; –Nonstandard‖ amino acids; Ionization equilibria of amino acids; Isoelectric point; Titration curve of amino acids

Unit 3: Protein structure **15 L**

Different levels of protein structure; Primary structure : polypeptide chains, disulfides and other cross-links; Secondary structures and their characteristics : α-helix, the β-sheet, π-helix, turns and loops and other secondary structures, peptide bond - torsion angles, Ramachandran plot, Helix breaker, Helical wheel; Supersecondary structures with examples; Domains; Motifs; Tertiary structures; Quaternary Structure; Protein data bank

Unit 4: Protein folding-Unfolding **15 L**

Protein stability – Electrostatic interactions, Ion-Dipole Interactions, Dipole-Dipole Interactions, Dipole-Induced-Dipole Interactions, Dispersion Forces, Empirical Potentials (Hard sphere potential, Lennard-Jones Potential), Force Fields, hydrogen bonding, hydrophobic forces-Accessible Surface Area, Molecular Nature, Temperature Dependence; Protein Denaturation-Renaturation, Anfinsen's experiment, Factors responsible for protein denaturation, Levinthal Paradox, Mechanisms of Protein Folding – different models, Molten globule state, Landscape theory – Folding funnel, Thermodynamics of protein folding; Folding accessory proteins – chaperones, Heat-shock proteins, GroEL/ES System; Protein structure prediction : The Chou–Fasman Method; Protein digestion – analysis of polypeptide chain and amino acid sequence; Post translational modifications

Unit 5: Other Biological macromolecules **5 L**

Membranes: lipid bilayer structure, Classification and properties of lipids; Nucleic acid: Nucleosides and Nucleotides, composition in DNA and RNA, Structural differences between RNA and DNA, Base pairing; Carbohydrates and sugars: Monosaccharides and Polysaccharides

Unit 6: Enzyme catalysis **5 L**

Catalytic Mechanisms - Michaelis-Menten Model, Significance of the Michaelis Constant, Inhibition - Competitive and Noncompetitive Inhibition, pH dependence

Unit 7: Experimental tools (5 out of the flowing listed) to study biological systems **15 L**

Principles and basic instrumentation of following techniques: UV-Vis spectroscopy**;** Circular dichroism spectroscopy**;** Sodium Dodecyl Sulfate Polyacrylamide Gel Electrophoresis**;** Micro calorimetry; X-ray Diffraction**;** Electron microscopy

References:

1. Nelson, D. L., Lehninger, A. L., & Cox, M. M. (2008). Lehninger principles of biochemistry. Macmillan.
2. Cantor, C. R., & Schimmel, P. R. (1980). Techniques for the study of biological structure and function.

3. Cantor, C. R., & Schimmel, P. R. (1980). Biophysical Chemistry, Part I: The Conformation of Biological Molecules. Journal of Solid-Phase Biochemistry, 5(3).

4. Voet, D., & Voet, J. G. (2010). Biochemistry. John Wiley & Sons.

Course Outcomes:

CO1: Students will get introduced to the field Biophysical Chemistry. Students will know the stereochemistry and chemical properties of different types of amino acids, their isoelectric points.

CO2: Students will know how to describe the protein structure at different levels.

CO3: Protein folding-unfolding process and their energy requirements will be studied here.

CO4: Students will get introduced to chemical compositions, structure and properties of other macromolecules such as lipids, carbohydrates.

CO5: Kinetics of enzymatic reactions will be studied here.

CO6: Students will learn different techniques to study biological processes, biomolecules.

CC 10: M.Sc. Chemistry Practical – III (Physical Chemistry)

Physical Chemistry II **Credits: 2**

(60 Lectures)

1. Conductometric experiments such as (at least one conductometric titration):

   a) Determination of Critical Micellar Concentration of surfactants

   b) Effects of external additives on CMC of surfactants

2. Spectrophotometric experiments:

Record UV—vis spectrum of a give compound (p-nitro phenol) in water and in presence of NaOH: Plot Absorbance/Transmittance vs. wavelength. Comment if there is any difference

3. Software based experiments such as (at least one):

   a) Visualization of protein structure by pymol software/chimera software

   b) Energy minimization by Gaussian software

4. pH-metric titration of polyprotic acid

5. Experiments on enzyme kinetics

6. Determination of the pI of an amino acid by titrimetric method

Course Outcomes:

CO1: Students will learn about physical experiments to determine physical parameters of molecules.

CO2: Students will be able to learn about predicting the lowest energy orbitals and processes through which energy minimization can also be predicted.

CO3: Apply molecular spectroscopy in structure elucidation of compounds which will help them not only in qualifying various competitive exams like NET, GATE etc, but also in the field of research.

Semester – III

CC-13: Physical Chemistry III:

Chemical Kinetics, Surface Chemistry and Macromolecules

(Credits: 4; Lecture – 04, Tutorial – 00, Practical - 00)

(60 Lectures)

Component: Theory **Physical Chemistry III** **Credits: 4**

Unit 1: Reaction Kinetics **25 L**

Collision Theory; Transition state theory; kinetic salt effects, steady state kinetics, Unimolecular reactions-Lindemann, Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theory.

Chain reactions; Fast reactions: flow method, relaxation method, flash photolysis; Oscillatory reactions; Autocatalysis; Electrode kinetics: Nernst, Butler-Volmer and Tafel equations. Kinetics of polymerization; step-growth vs. chain-growth polymerizations

Unit 2: Interfacial Chemistry **10 L**

Surface Chemistry; Curved surfaces: Young-Laplace and Kelvin equations. Adsorption of solids: BET equation. Micelles, reverse micelles; micellization equilibrium and its thermodynamics; Emulsions.

Unit 3 : Solid State **10 L**

Band theory of solids, conductors, semiconductors (n-type, p-type and n-p junction), superconductors and insulators. Lattice defects (Schottky defect and Frenkel defect). Color centre: F-centre, V-centre, F′-centre etc.

Unit 4: Macromolecules **10 L**

Molecular weight determination of polymers by different methods, such as: viscometry, osmometry, light scattering, chromatography and ultracentrifugation methods; Kinetics of polymerization; step-growth vs. chain-growth polymerizations

Unit 5: Introduction to Nanoparticles **5 Lectures**

Scope and importance of nanoscience and nanotechnology. Overview of nanomaterials and naoparticles: Definition to nanomaterials, Optical properties-absorption, emission; semiconductor and Plasmonic NP; Surface energy, Magnetic properties; Mechanical / Frictional properties; Electrical Transport properties.

References :

1. Chemical Kinetics – K.J.Laidler
2. Physical Chemistry of Macromolecules – C. Tanford
3. Physics and Chemistry of Surfaces – N.K. Adams
4. Solid State Chemistry & Its Application – A. R. West
5. Introduction to Solid State Theory – O.Madelung
6. Physical Chemistry of Surfaces – A.W. Adamson

Course Outcomes:

CO1: Students will learn about reaction kinetics theories of complex multi-step reactions.

CO2: Kinetics of catalytic reactions as well as those in electrochemical cells will also be learned.

CO3: Students will gain knowledge of about chemistry on surfaces and interfaces. This is in directly related to the colloids, emulsions and micelle solutions used in daily life.

CO4: Students will learn about structure and physical parameters of different matters (conductors, semiconductors, insulators) in solid state. The parameters viz. band gap, defects etc are in direct consequence with their physical properties e.g. electrical conductivity, magnetic property.

CO5: Students will get introduced to fundamental aspects of nanomaterials.

CO6: Students will study kinetics of polymerization reactions, methods of determinations of average molecular weights of polymers using different techniques.

CC-14 : Polymer Chemistry and Nanotechnology

Component: Theory **Credit: 4**

(Credits: 4; Lecture – 04, Tutorial – 01, Practical - 00)

(**60 Lectures**)

Unit 1. : Classification and configuration of polymers **10L**

Definition and Classification of polymers; natural, semisynthetic and synthetic polymers; Linear, branched and crosslinked polymers; Homo polymers and copolymers. Graft and block copolymers, elastomers, fibres, plastics, thermoplastic and thermosetting polymers. Tacticity in polymers-Isotactic, syndiotactic and atactic polymers. Properties of polymers : Glass transition temperature (Tg) - Definition- Factors affecting Tg - relationships between Tg and molecular weight and melting point. Importance of Tg. composites, blends.

Unit 2. : Polymerisation Techniques and Application of polymers **20L**

Types of polymerization- addition (initiation, propagation and termination), condensation, ionic (cationic & anionic), Ring opening polymerizations (epoxy resins) coordination polymerization – 65 Ziegler Natta catalyst; biodegradable polymers. Properties and applications of - Plastics: Polyethylene, Polyvinylchloride, polymethyl methacrylate, Teflon. Rubbers: natural and synthetic rubbers –nitrile rubber, BUNA-S, BUNA N, neoprene rubber; Vulcanization of rubber. Synthetic fibres : Nylon 66, Nylon 6. Polymers in medical field, adhesive and coatings, Environmental Hazards of plasticsand recycling.

Unit 3 : Conducting Polymers **10L**

Conducting Polymers (CP) : Unique properties of CP. Preparation and properties of Polyaniline and Polypyrrole. Concept of Doping and application of CP in Chemical and Biosensor, antistatic coating, display and LED.

Unit 4 : Nanotechnology **10L**

Nano versus bulk, quantum confinement, Classification of nanoparticles (NPs) according dimensions: 0D, 1D and 2D nanoparticles - definitions and examples. Classification of nanoparticles (NPs) according to its composition: metallic, oxide, sulfide, carbon nanoparticles, nanocomposites and also other types.

Methods of nanoparticles synthesis — Top-down & Bottom-up methods: Chemical precipitation and co-precipitation, sol-gel methods, microemulsions or reverse micelles techniques.

Unit 5: Applications of Nanomaterials **10 Lectures**

Applications in solar energy conversion and catalysis: Quantum dots for solar cells, Quantum dots for light emitting diode, Molecular electronics, Photovoltaic, fuel cells, batteries and energy-related applications High strength nanocomposites, Nanoenergetic materials, nanoelectronics, topological insulator.Nanoparticles as catalysts; Applications of one dimensional nanotubes and nanowires.Nanomaterials for biological and environmental applications: Nanoparticles-Drug delivery systems & Controlled Release, Targeted-Ligand Applications in Drug Delivery Systems, Cancer Therapy, Nanosystems in Inflammation, Targeting Macrophages to Control Inflammation, Tissue Regeneration, Growth and Repair, Tissue Bioengineering, Impact of Drug Discovery and Development.

Course Outcomes:

CO1: Students will learn the definition and different classifications of polymers, molecular weight measurement techniques; structure and stereochemical classifications of polymers will also be studied.

CO2: Students will learn about different polymerization techniques, their characteristics, kinetics and specific reaction conditions. Different initiators and their effect on polymerization will also be learned.

CO3: Glass Transition Temperature (Tg) and Classification of polymers based on Tg will be learned. Properties of different polymers rubber, plastics and thermosets and their relation with glass transition temperature will also be learned. Crosslinking of polymers, IPN and Gel will also be studied in this course.

CO4: Preparation, properties and Applications of some common polymers (Polyethylene, Polyvinylchloride, polymethyl methacrylate, polyethylene terphthatalate, Teflon, Bakelite. Rubbers: natural and synthetic rubbers, Synthetic fibres: Nylon 66, Nylon 6, Rayon etc) will be studied.

CO5: Origin of Biodegradability in polymers, approach towards synthesis of Biodegradable polymers, their properties and applications in different fields will be studied.

CO6: Advanced topics of polymer science viz. conducting polymers, liquid crystal polymers etc are studied in this course. Special properties of these polymers and their unique applications are also learned and understood accordingly. Students will also learn the basics of nanotechnology and application of nanoparticles / nanomaterials in different sectors.

CC-15: MSc Practical VI (Physical Chemistry)

Physical Chemistry III **Credits: 2**

1. Preparation of silver nanoparticles and characterization
2. Fluorimetric experiment such as:
   i. To study the fluorescence behaviour of tryptophan in polar and non-polar media
   ii. Experiment on Stern-volmer constant using steady state fluorescence
3. Determination of molecular weight of a high polymer (e.g. PEG) by viscosity measurement.
4. Potentiometric titration such as
   i. Potentiometric titration of halide mixture
   ii. Determine the E^0 value of Ag^+/Ag electrode and activity coefficients of different aqueous $AgNO_3$ solutions potentiometrically
   iii. Determine the standard potential of $[Fe(CN)_6]^{3-}$/ $[Fe(CN)_6]^{4-}$ electrode by potentiometer
5. Conductometric titration such as
   i. Verify the Onsagar equation using KCl, K_2SO_4 and $BaCl_2$ as electrolytes and determine their Λ_0 values
   ii. Determination of dissociation constant and Λ_0 of a weak monobasic acid conductometrically and verification of Ostwald's Dilution Law
   iii. Conductometric determination of concentrations of KCl, HCl and NH_4Cl in a mixture
   iv. Determine the solubility product of $BaSO_4$
6. Spectrophotometric experiment

i. Study the kinetics of Iodination of acetone spectrophotometrically

ii. Determination of composition of complexes (Ferric-salicylate complex/Ferrous-orthophenanthroline complex) by Job's method.

Course Outcomes:

CO1: Interpret and identify the fusion behavior of different inorganic compounds.

CO2: Develop skill on fusion test of different metal oxides.

CO3: Illustrate the analysis of unknown Inorganic samples.

CO4: The student will learn how to use equipments like potentiometer and conductometer for physical characterization.

CO5: The student will learn the basics of colloidal chemistry.

CO6: The student will learn how to use absorption and fluorescence spectroscopic techniques for chemical applications.

<u>Semester – IV</u>

CC – 16: Chemistry Master Project & Dissertation

Chemistry Master Project & Dissertation **Credit: 20**

A research project work should be done individually under the guidance of one (or more) faculty of Chemistry department at SNU or anywhere else on any topic related to the subject & can be recorded as dissertation & also be presented by the candidate in front of external and internal examiners in a seminar presentation. Project may be divided into two parts: the first part (of credit 04) would be carried out after second semester for one month. The second part (of credit 04) would be carried out during fourth semester.