

# **FACULTY OF SCIENCES**

## **SYLLABUS**

**for**

### **M.Sc. (Hons. School) Chemistry**

**(Under Credit Based Continuous Evaluation Grading System)**

**(SEMESTER: I - IV)**

**Examinations: 2016-17**



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## **GURU NANAK DEV UNIVERSITY AMRITSAR**

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M.Sc. Chemistry (Hons. School) (Semester System)  
(Under Credit Based Continuous Evaluation Grading System)

**FIRST SEMESTER:**

<b>Sr. No.</b>	<b>Course No.</b>	<b>Course Title</b>	<b>Credit L-T-P</b>
1	CYL402	Organometallics	4-0-0
2	CYL403	Organic Synthesis-III	3-0-0
3	CYL404	Structure Elucidation of Natural Products	3-0-0
4	CYL405	Chemical Kinetics	3-0-0
5	CYL406	Physical Chemistry	3-0-0
6	CYL415	Electrochemistry	3-0-0
7	CYP401	Organic Synthesis	0-0-3
8	CYP402	Physical Chemistry	0-0-3

**SECOND SEMESTER:**

<b>Sr. No.</b>	<b>Course No.</b>	<b>Course Title</b>	<b>Credit L-T-P</b>
1	CYL411	Cluster and Cage compounds	3-0-0
2	CYL412	Spectral Techniques in Inorganic Chemistry	3-0-0
3	CYL413	Biosynthesis of Natural Products	3-0-0
4	CYL414	Spectroscopy in Structure Elucidation and Asymmetric Synthesis	3-0-0
5	CYL416	Physical Chemistry	3-0-0
6	CYL417	Green Chemistry	3-0-0
7	CYP411	Inorganic Chemistry	0-0-3

M.Sc. Chemistry (Hons. School) (Semester System)  
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**THIRD SEMESTER:**

Sr. No.	Course No.	Course Title	Credits
1	CYL501	Inorganic Chemistry	3-0-0
2	CYL502	Photochemistry and Pericyclic Reactions	3-0-0
3	CYL503	Chemistry of Materials	3-0-0
4		Interdisciplinary Course-I	4-0-0
5		Interdisciplinary Course-II	4-0-0
		Dissertation (to be continued in semester 4 <sup>th</sup> )	15-0-0

**FOURTH SEMESTER:**

Sr. No.	Course No.	Course Title	Credits
1	CYL504	Inorganic Chemistry	3-0-0
2	CYL505	Bio-organic Chemistry	3-0-0
3	CYL506	Bio-physical Chemistry	3-0-0
4	CYP 507	Dissertation (continued from Semester 3 <sup>rd</sup> )	15-0-0

Dissertation is to be submitted by 31<sup>st</sup> March in 4<sup>th</sup> semester. The viva examination will be completed before the theory examinations.

**Optional Courses**

**Choose any one course**

5	CYL566	Organic Chemistry-V Advanced Organic Synthesis	4-0-0
6	CYL570	Inorganic Chemistry-VII (Bioinorganic Chemistry)	4-0-0
7	CYL571	Inorganic Polymers	4-0-0

**CYL402: Organometallics**

**Credit: 3-0-0**

**1. Introduction**

**2. The 18 Valence Electron Rule:** Introduction, The 18 electron rule, counting of electrons and finding metal-metal bonds and related problems.

**3. Alkyl, Aryl and Ligands with Higher Hapticity:**

- (i) Sigma bonded alkyl groups as ligands: Synthesis of metal-alkyl compounds,  $\beta$ -hydride elimination,  $\pi$ -bonded  $\eta^1$ -aryl ligands.
- (ii) Cyclic and acyclic polyenyl  $\pi$ -bonded ligands: Cyclopentadienyl ( $Cp^-$ ), Synthesis of Cp based sandwich compounds, Structure and properties of  $MCp_2$  complexes, The first metal-sandwich compound Ferrocene, Reactions of metal-sandwich compounds, Bent sandwich compounds, Schwartz reagent and hydrozirconation, Chemistry of  $Cp^*$ , Chemistry of arene sandwich compounds, Allyl groups as ligands, 1,3-Butadiene complexes, Cyclobutadiene complexes, Cycloheptatriene and Cyclooctatetraene as ligands. Davies-Green-Mingos (DGM) rules.
- (iii) Ferrocene: Structure and bonding of ferrocenes, Basic chemical reactions of Ferrocene, Reactions of Acetyl Ferrocene and formyl Ferrocene, lithiated ferrocenes and their reactions, (Dimethylaminomethyl)Ferrocene and its methiodide salt, Ferrocene boronic acid and haloferrocenes, Chirality in Ferrocene derivatives, Synthesis of chiral Ferrocene based compounds, Ferrocene based condensation polymers.
- (iv) Recaptulation of Metal carbonyls.

**4. Applications of Organometallic Complexes to Catalysis:**

Catalysis, Terminology in catalysis, sequences involved in a catalysed reaction, asymmetric synthesis using a catalyst, Hydrogenation catalysts, classification of hydrogenation catalysts, catalytic cycle of Wilkinson's catalyst, catalytic cycles of iridium and ruthenium based catalysts, hydrogenation by lanthanide organometallic compounds, catalytic asymmetric synthesis, Hydroformylation: Cobalt catalysts and phosphine modified cobalt catalysts, Rhodium-phosphine catalysts, factors affecting the n/iso ratio of hydroformylation products; Methanol Carbonylation and Olefin Oxidation: Monsanto, Cativa and Wacker Processes,; Polymerisation and oligomerisation of olefins and dienes, carboxylation of olefins, carbonylation of methanol, Synthetic gas.

**5. Bioorganometallic Chemistry:**

Role of organometallics in heavy metal poisoning: Mercury and Arsenic poisoning, organometallic compounds as drugs: ruthenium and ferrocene based drugs; Organometallics as radiopharmaceutical, tracers, ionophores and sensors.

**Books Recommended:**

1. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Inter-Science.
2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Inter-Science.
3. B.D. Gupta and A.J. Elias, Basic Organomettallic Chemistry, Universities Press.
4. C.E.A. Salzer and E. Elchinbroich, Organometallics, A Concise Introduction Chemistry, VCH.

**CYL403: Organic Synthesis – III**

**Credit: 3-0-0**

**1. Addition to Carbon-Hetero Multiple Bonds**

**14 Hrs**

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

Hydrolysis of esters and amides, ammonolysis of esters.

**2. Elimination Reactions**

**5 Hrs**

The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

**3. Oxidation**

**7 Hrs**

Introduction. Different oxidative processes.

Hydrocarbons- alkenes, aromatic rings, saturated C-H groups activated and unactivated. Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids.

Amines, hydrazines, and sulphides.

Oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate.

**4. Reduction**

**7 Hrs**

Introduction. Different reductive processes.

Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings.

Carbonyl compounds – aldehydes, ketones, acids and their derivatives. Epoxides.

Nitro, nitroso, azo and oxime groups.

Hydrogenolysis.

**5. Rearrangements**

**12 Hrs**

General mechanistic consideration – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements, Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction.

**Recommended Books:**

1. Organic Reaction Mechanism by Jerry March, John Wiley Ed. 5, 2002.
2. Advanced Organic Chemistry by Francis Carey, Vol. A and Vol. B

**CYL404: Structure Elucidation of Natural Products**

**Credit: 3-0-0**

**Terpenoids and Carotenoids:**

**10hrs.**

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination and synthesis of citral, geraniol, camphor, farsenol, santonin, abetic acid.

**Alkaloids:**

**10hrs.**

Definition, nomenclature and physiological action, occurrence, isolation, general methods of elucidation, degradation, classification based on nitrogen heterocyclic ring, Structure, stereochemistry, synthesis of ephedrine, nicotine, atropine, morphine.

**Steroids:**

**10hrs.**

Occurrence, nomenclature, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, bile acids, Androsterone, testosterone, estrone, progesterone.

**Disconnection approach:**

**12hrs**

An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

**Protecting groups:**

**3hrs.**

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

**Books:**

1. Designing Organic Synthesis, S. Warren, Wiley
2. Organic synthesis- Concepts, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlag VCH.
3. Advanced Organic Synthesis Part B, F.A. Carey and R. J. Sundberg, Plenum Press.
4. Principles of Organic Synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
5. Organic Chemistry by I. L. Finar, Vol. 2.

### **CYL405: Chemical Kinetics**

**Credit: 3-0-0**

#### **UNIT – I**

**Basic Kinetic Concepts :** Chemical kinetics and its scope. Order & molecularity. Rate constants and rate coefficients. Rate laws. Factors affecting rates: concentration, temperature, pressure, solvent, light, catalyst.

**Methods of Determining Rate Laws:** Differential method, method of integration, First order, Second order and Third order reactions with examples, half lives, pseudo-molecular reactions, isolation method, reaction of nth order, comparison of methods.

**Influence of Temperature on Reaction Rates:** Arrhenius equation, Improved treatments of temperature, pressure, solvent, light, catalyst.

**Experimental Methods of Chemical Kinetics :** Conductometric, potentiometric, optical methods, polarimetry and spectrophotometer.

**Kinetics of Reactions:** Reversible or opposing reactions. Consecutive or series reactions, Parallel reactions.

**Theory of Reaction Rates:** The Collision theory of bimolecular reactions based on hard sphere model. Steric factor. Lindemann's mechanism. The transition state theory. Thermodynamic treatment and statistical mechanical approach. Eyring treatment. Transmission coefficient. Tunneling effect. Kinetic theory of termolecular reactions.

#### **UNIT-II**

**Elementary Gas-phase Reactions:** Lindemann- Christiansen hypothesis. Hinshelwood's treatment. Rice-Ramsperger-Kassel (RRK) treatment. Slater's treatment. Rice-Ramsperger-Kassel Marcus (RRKM) treatments of unimolecular gas phase reactions.

**Reactions in Solutions:** Factors affecting reactions in solutions. Ionic reactions in solutions. Effect of solvent. Effect of ionic strength. Primary and Secondary salt effects.

**Composite/Complex Reactions:** Types of composite mechanisms. Rate equations for composite mechanisms. Simultaneous and Consecutive reactions. Steady-state treatment. Rate-determining (Rate- controlling) steps. Microscopic reversibility and detailed balance.



### UNIT-III

**Homogeneous Catalysis:** Catalysis. Character of catalyst. Simple catalysed reactions. Kinetics of acid-base catalysis; General acid base catalysis. Mechanisms of acid-base catalysis. Catalysis by enzymes; Influence of substrate concentration, Influence of pH, Influence of temperature. Transient - phase kinetics.

**Reaction in Flow Systems:** Techniques for very fast reactions. General features of fast reactions. Stopped-flow method. Relaxation methods. Shock tube methods. Flash photolysis. Nuclear- magnetic resonance methods.

**Kinetics of Dynamic Chain Reactions:** Hydrogen- bromine reactions. Hydrogen- chlorine reaction. Pyrolysis of acetaldehyde. Organic decomposition; Decomposition of ethane.

**Photochemical Reactions:** Hydrogen- bromine reactions. Hydrogen-chlorine reactions.

**Oscillatory Chemical Reactions:** Belousov-Zhabotinsky reactions. Classification of Oscillatory reactions.

#### Books Recommended:

1. Chemical Kinetics, K.J. Laidler.
2. Kinetics and Mechanism, A.A. Frost & R.G. Pearson.
3. Comprehensive Chemical Kinetics, C/H Bam Ford & C.F.H. Tipper.
4. Principles of Physical Chemistry, S.H. Maron & C.F. Prutton.
5. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose.

**CYL406: Physical Chemistry**

**Credit: 3-0-0**

**1. Thermodynamics (15 Hrs):**

Thermodynamics of ideal and non-ideal mixtures, excess functions.

Activity, activity coefficients and their determination: Standard states and reference states for a solute and solvent. Determination of activities from vapour pressure, freezing point, boiling point, E.M.F. measurements, osmotic pressure. Solutions of Electrolytes. Mean activities of electrolytes, determination of activities for electrolytes from freezing point, boiling point, osmotic pressure, E.M.F. and solubility measurements. Debye-Huckel treatment of dilute electrolyte solutions.

**2. Micelles (15 Hrs):**

Surface active agents, classification of surface active agents, micellization, micelle structure and shape, shape transitions, elongated micelles, vesicles, inverted structures, micelle aggregation number, hydrophobic interaction, critical micelle concentration (CMC), factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization,  $G$ ,  $H$ ,  $S$  of micelle formation, phase separation, and mass action models, solubilization, microemulsion, nanoemulsions, reverse micelles. Micellar catalysis, Gemini surfactants.

**3. Nano-chemistry and Synthesis of Nanomaterials (15 Hrs):**

An introduction to nanochemistry, synthesis of nanomaterials: Metal nanocrystals by reduction, solvothermal synthesis, photochemical synthesis, electrochemical synthesis, nanocrystals of semiconductors and other materials by arrested precipitation, nanochemical routes. Solvated metal atom dispersion, sol-gel, self-assemblies, self-assemblies, self-assembling Block copolymers.

**Books Suggested:**

1. Physical Chemistry by Atkins.
2. Surfactants and Interfacial Phenomena by M.J. Rosen.
3. Physical Chemistry by Maron and Prutton.
4. Thermodynamics for Chemists by S. Glasstone.
5. Concepts of Nanochemistry by L. Calemartiri and G. A. Ozin.
6. Nanochemistry : A Chemical Approach to Nanomaterials by G.A Ozin and A. Arsenault.

**CYL415: Electrochemistry**

**Credit: 3-0-0**

**1. The Electric and Magnetic Properties (15 Hrs):**

Electric properties of molecules, permanent and induced electric dipole moments, intermolecular forces, interactions between dipoles – repulsive and total interactions. Molecular interactions in beams, scattering effects, paramagnetic, diamagnetic, magnetic susceptibility, gouy balance, permanent magnetic moment, induced magnetic moments.

**2. Electrochemistry of Solutions (20 Hrs):**

Ion-solvent interactions, the Born model, electrostatic potential at the surface of a charged sphere, Born expression for the free energy of ion-solvent interactions, structural treatment of ion-solvent interactions, ion-dipole moment, evaluation in the ion-dipole approach to heat of solvation, solvation number, static and dynamic pictures of ion-solvent interactions, hydration number, dielectric constant of water and ionic solutions, relation between dielectric constant and internal counter fields. Debye equation for dielectric constants between dipoles on the average effective moment of polar, dielectric constant of liquids containing associated dipoles, ion – solvent nonelectrolyte interactions, change in solubility of non-electrolyte due to primary and secondary solvations.

**3. Dynamic Electrochemistry (10 Hrs):**

Electrochemical cell reactions, Nernst equation, the rate of charge transfer, the activation Gibbs's energy, the Butler – Volmer equation, the low and high overpotential limits, polarization, electrode kinetics, electrical double layer, electrode/electrolyte interface, batteries, primary, secondary fuel cells, corrosion and corrosion prevention.

**Books Suggested:**

1. Electrochemistry by Bockris.
2. Physical Chemistry by Atkins.

**CYP401: Organic Synthesis Lab**

**Credit: 0-0-3**

The use of multi-step approach in organic synthesis and applications of spectroscopic techniques to determine the structures of the compounds prepared.

1. Synthesize (a) 2,4-dinitro-1-chlorobenzene from chlorobenzene, (b) mixture of o- and p-nitrophenols from phenol and (c) p-nitroacetanilide from acetanilide and make comparison of the reactivities of various substrates and reaction conditions used for performing nitration in each experiment. (book 2, pp978-979, 919-20)
2. Synthesis of 2-chloro-4-bromo-6-iodoaniline from aniline. (Book 1, pp 292-299)
3. Synthesis of benzalacetophenone by condensation of benzaldehyde with acetophenone. and study its bromination and subsequent debromination. (Book 1, pp 242-247, book 3 pp 361-365)
4. The epoxidation of benzalacetophenone to its epoxide and study its reactivity towards hydroxyl ion. (Book 3, pp 363-364).
5. Michael addition of aniline to benzalacetophenone. (Book 1, p 247)
6. Conversion of benzalacetophenone to its oxime and its transformation to amide and oxazole derivatives. (Book 1, pp 242-247, book 3 pp 361-365)
7. Synthesis of anthranilic acid from phthalimide. (Book 2, pp 898-899)
8. Synthesis of p-aminobenzenesulfonamide. (Book 1, pp 275-289)
9. Synthesis of Methyl n-pentyl ketone from ethyl acetoacetate. (Book 2, pp 620-621)
10. Synthesis of triphenylcarbinol from bromobenzene. (Book 2, pp 540-541)

**Suggested Books:**

1. An introduction to Modern Experimental Organic Chemistry, R.M. Roberts, J.C. Gilbert, L.B. Rodewald and A.S. Wingrove. Holt, Rinehart and Winston Inc., New York. 1969.
2. Vogel's Text book of practical organic chemistry, 5<sup>th</sup> Edition.
3. Laboratory Experiments in Organic Chemistry, R. Adams, J.R. Johnson and C.F. Wilcox, The Macmillan Limited, London, 1970.

**CYP402: Physical Chemistry Lab**

**Credit : 0-0-3**

**A) Conductometry:**

- 1). Determine the basicity of organic acids (Oxalic/benzoic acid).
- 2). Study the effect of solvent on the conductance of  $\text{AgNO}_3$ /Acetic acid and determine the degree of dissociation and equilibrium constant in different solvents and in their mixture (DMSO, DMF, dioxane, acetone, water) and test the validity of Debye-Huckel-Onsager's theory.
- 3). Determine the degree of hydrolysis and hydrolysis constant of  $\text{CH}_3\text{COONa}/\text{NaCl}$ /aniline hydrochloride.
- 4). Titration of a mixture of  $\text{HCl}$ ,  $\text{CH}_3\text{COOH}$  and  $\text{CuSO}_4$  with  $\text{NaOH}$ .

**B) pH metry:**

- 5). Determine pH of a number of solutions containing  $\text{CH}_3\text{COOH}$  and  $\text{CH}_3\text{COONa}$  and hence dissociation constant of the acid.
- 6). To determine acid and base dissociation constants of amino acid.

**C) Colorimetry:**

- 7). Study the complex formation between Nickel and o-phenanthroline.
- 8). Determine pK value of an acid-base indicator (Methyl red).
- 9). To determine the stability constant of a charge transfer complex.
- 10). Simultaneous estimation of  $\text{Mn}^{2+}$  and  $\text{Cr}^{3+}$  in a solution of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$ .

**D) Chemical Kinetics:**

- 11). Study the salt effects and the solvent effect on the rate law of alkaline hydrolysis of crystal violet.
- 12). To determine the rate constant of a reaction between  $\text{K}_2\text{S}_2\text{O}_8$  and  $\text{KI}$  at two temperatures and hence determine the activation energy.

**E) Thermodynamics:**

- 13). Study the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interaction (benzoic acid in water and DMSO-water mixture). Calculate the partial molar heat of solution.
- 14). Determine the partial molar volume of Glycine/ $\text{NaCl}$ /Methanol/Urea in  $\text{H}_2\text{O}$  using dilatometer.

M.Sc. Chemistry (Hons. School) Semester – I  
(Under Credit Based Continuous Evaluation Grading System)

- 15). Determine the molar refractivity for water and DMSO/DMF/acetone/dioxane and their mixtures and verify the additivity rule. Predict about the interaction between two compounds of mixture by plotting refractive indices vs. mole fraction.

**F) Refractometry:**

- 16). Determine the refractive indices of different solutions of given electrolyte (say KCl) and hence determine the composition of unknown solution of the salt.  
Or

**Determine the molar refractivity for water and DMSO/DMF/acetone/dioxane and their mixtures and verify the additivity rule. Predict about the interaction between two compounds of a mixture by plotting  $n$  vs. mole fraction.**

**G). Phase Rule:**

- 17) Draw the phase diagram for any one of the following three component partially immiscible liquid systems. DMSO-water-benzene, water-benzene-acetic acid, Acetone-water-EMK.

**H). Potentiometry:**

- 18) To calculate thermodynamic parameters as  $G$ ,  $S$  and  $H$  for the reaction  
$$\text{Zn} + \text{Hg}_2\text{SO}_4 \rightleftharpoons 2\text{Hg} + \text{ZnSO}_4$$
 by e.m.f. data.

**I). Polarography:**

- 19). Estimation of ions in mixture of  $\text{Pb}^{2+}$  and  $\text{Cd}^{2+}$  by successive reduction Evaluate diffusion coefficient of  $\text{Cd}^{2+}$ .

**Books Recommended:**

1. Findlay's Practical Physical Chemistry.
2. Advanced Practical Physical Chemistry by J. B. Jadav.
3. Quantitative Inorganic Analysis by Vogel.

**CYL411: Cluster and Cage compounds**

**Credit: 3-0-0**

**(45 hrs.)**

**1. Chains (5Hrs):**

Catenation, heterocatenation, zeolites, intercalation chemistry, one-dimensional conductors.

**2. Rings (5Hrs):**

Borazines, Phosphazenes (synthesis, bonding & reactions), Phosphazene polymers homocyclic inorganic systems.

**3. Cages (10Hrs):**

Introduction, boranes, *styx* numbers, bonding problems in Boranes, Chemistry of boranes-reaction with Lewis bases, Borane cages, B<sub>12</sub>H<sub>12</sub> and other boranes derived from B<sub>12</sub>H<sub>12</sub>, structure relationship of closo, nido, archano and hypo boranes, heteroboranes, carboranes, metallocarboranes, structure prediction of heterocarboranes. Cage compounds having phosphorus oxygen, phosphorus and sulphur .

**4. Cluster Compounds (15 hrs.)**

Cluster compounds, molecular structures of clusters metal carbonyl clusters, stereochemical nonrigidity in clusters, Electronic structures of clusters with  $\pi$ -acid ligands, electron counting schemes for HNCCs, the capping rule, structures not rationalized by PESPT model, isoelectronic and isolobal relationship, high nuclearity carbonyl clusters (HNCCs) (Structure patterns, synthesis methods), heteroatoms in metal atom clusters: carbide and nitride containing clusters, HNCCs of Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt etc.

**5. Lower Halide and Chalcogenide Clusters (5 Hrs.):**

Octahedral metal halide and chalcogenide clusters (M<sub>6</sub> X<sub>8</sub> and M<sub>6</sub> X<sub>12</sub> types), Chevrel phases, triangular clusters and solid state extended arrays.

**6. Compounds with M-M multiple bonds : (5 Hrs.)**

Major structural types, quadrupole bonds, other bond orders in tetragonal context, relation of clusters to multiple bonds.

**Recommended Books:**

1. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley & Sons, Inc., New York., 1994.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry, 4th Edn., Pearson Education, Singapore, 1999.
3. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 5th or 6th Edition Interscience Publishers.

**CYL412: Spectral Techniques in Inorganic Chemistry**

**Credit: 3-0-0**

**1. Nuclear Quadruple Resonance Spectroscopy (10 Hrs.):**

Introduction, experimental considerations, fundamentals of NOR spectroscopy, origin of EFG, measurement of energy differences between two nuclear spin states, the asymmetry parameter, effects of the magnetic field, interpretation of the spectra, application of the technique to halogen compounds, group, elements, transition metals, complications in the spectra. (book 1,2).

**2. Mossbauer Spectroscopy (10 Hrs.)**

Experimental considerations, the spectrum and its parameters, simple spin states ( $1/2$ ,  $3/2$ ), higher spin states ( $I > 3/2$ ), magnetic splitting significance of parameters obtained from spectra, quadrupole splitting, additive model, interpretation of Mossbauer spectra of  $^{57}\text{Fe}$ ,  $^{119}\text{Sn}$ , (book 1,2).

**3. Electron Paramagnetic Resonance Spectroscopy (15 Hrs.):**

Introduction, principle, Presentation of spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, EPR spectrum of benzene radical anion, methylcyclopentadienyl radical, pyrazine anion, pyrazine anion with  $^{23}\text{Na}$  and  $^{39}\text{K}$  counter ion, Nitrosyl nitroxide, factors affecting magnitude of g values, zero field splitting and Kramer's degeneracy, Qualitative survey of EPR spectra of first row transition metal ion complexes ( $d^1$ ,  $d^2$ ,  $d^3$ , low spin  $d^5$ ,  $d^5$ , high spin  $d^6$ ,  $d^7$ ,  $d^9$  system). (book 1,2).

**4. Nuclear Magnetic Resonance: (15 Hrs.)**

Recapitulations, NMR of inorganic compounds,  $^1\text{H}$  NMR of organometallics- chemical shift, coupling effects, phosphorous and arsine ligands, transition metal hydrides, coupling to phosphine ligands, coupling to metal, effect of trans ligand, introduction to isotopes other than  $^1\text{H}$  e.g.  $^{31}\text{P}$ ,  $^{13}\text{C}$ ,  $^{14}\text{N}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ . (books 1, 2 & 3)

**5. Magnetic Properties of Transition Metal Ions: (10 Hrs.)**

Van Vleck's formula for susceptibility, first order Zeeman effect, second order Zeeman effect, KT states, quenching of orbital angular momentum by ligand field, magnetic properties of A and E terms, electronic delocalization, magnetic properties of  $d^n$  and  $f^n$  metal ions.



**Books Recommended:**

1. R. S. Drago, Physical Methods in Chemistry, W.B. Saunders Company.
2. R.V. Parish, NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, Eds Elis Horwood.
3. E.A.V. Ebsworth, D.W.H. Rankin and S.J. Cradock, Structural Methods in Inorganic Chemistry, Blackwell Scientific, Oxford, 1987.
4. A. Earnshaw, Introduction to Magnetochemistry, Academic press.
5. Syamal and Dutta, Magnetochemistry

**CYL413: Biosynthesis of Natural Products**

**Credit: 3-0-0**

1. **Introduction:** **4 Hrs**  
 Functions of metabolism. Primary and secondary metabolism. Biochemical reactions and organic reaction mechanisms. Principle Pathways and technique of elucidation metabolic sequences. The one carbon fragment.  
**Primary Metabolism:** **10 Hrs**  
 General introduction to catabolic and anabolic pathways. Regulation of metabolic pathways. Structure and functions of ATP, free energy of hydrolysis of ATP. Photosynthesis. Carbohydrate metabolism-Glycolysis, Citric acid cycle, Glycogenesis Glycogenolysis and Glyconeogenesis, pentose phosphate Pathway. Electron Transport System and Oxidative Phosphorylation.
3. **Secondary Metabolism:**
  - a) **Metabolites Derived from Acetate (Polyketide Pathway):** **6 Hrs**  
 Biosynthesis of unsaturated and saturated fatty acids, prostaglandins, polyphenols viz. Orsellinic acid, 6-methylsalicylic acid, usnic acid, penicillic acid, patulin, citrinin, griseofluvin, alizarin, emodin, tetracyclines.
  - (b) **Metabolites Derived from Mevalonic Acid Pathway (Terpenes):** **10 Hrs**  
 Biosynthesis of mevalonic acid and the active isoprene units, monoterpenes viz. Citral, geraniol, pinene, camphor, terpineol, thujone, isobornylene, menthol, artemesia alcohol, santolina alcohol, Iridoids, viz. Loganin, iridomyrmecin, secolaganin, sweroside. Sesquiterpenes, viz. Humulene,  $\alpha$ -cedrene,  $\gamma$ -bisabolene, ovalicin, juvenile hormone, Diterpenes, viz. Phytol, Sclareol, abietic acid, taxinine. Triterpenes, squalene, lanosterol, cholesterol, cycloartenol, sitosterol, Vitamin D. Biological functions of steroids. Biosynthesis of carotenoids, viz.  $\alpha$ -carotene,  $\beta$ -carotene, vitamin A.
  - (c) **Metabolite Derived from Shikimic Acid Pathway:** **4 Hrs**  
 Biosynthesis of shikimic acid, aromatic amino acids, cinnamic and benzoic acid, coumarines.
  - (d) **The Alkaloids :** **6 Hrs**  
 Biosynthesis of coacin, tropine, pseudopelletierine, coniine, nicotine, sparteine, ephedrine, morphine, quinine.
4. **Amino Acids, Peptides and Proteins:** **5 Hrs**  
 Introduction, amino acid classification and structure, chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding secondary structures.  $\alpha$ - helix and  $\beta$ -sheet. Tertiary structure of protein folding. Quaternary structure. Biosynthesis of amino acids.

**Books:**

1. Primary Metabolism: a Mechanistic Approach by J. Staunton, Oxford University Press, 1978.
2. Secondary Metabolism by J. Mann, Oxford University Press, Oxford, 1980.
3. Natural Product Chemistry - A Mechanistic, Biosynthetic and Ecological Approach by Kurt B. G. Torrsell, Swadish Pharmaceutical Society, 1997.
4. Principles of Biochemistry by A. L. Lehninger, CBS Publishers, New Delhi.
5. Fundamental of Biochemistry by D. Voet, J.G. Voet and C.W. Pratt, John Willey & Sons Inc., New York, 1999.

**CYL414: Spectroscopy in Structure Elucidation and  
Asymmetric Synthesis**

**Credit: 3-0-0**

**1. Asymmetric Synthesis 20 lectures**

**General Aspects: 3 lectures**

Analytical methods for determination of enantiomeric purity – GC, HPLC and NMR. Natural sources of chiral starting materials, classification and methods of formation of new chiral compounds.

**Non-enzymatic Approaches 10 lectures**

Methods of asymmetric synthesis using naturally occurring chiral compounds, nucleophile and electrophile bearing chiral auxiliary, Diels – Alder cycloaddition and Claisen – cope rearrangements.

Asymmetric carbon – carbon bond formation using alkylation, Michael reaction and addition to carbonyl compounds. Cram's rule and Felkin – Ahn model. Asymmetric oxidation and reductions.

**Enzymatic Approaches: 7 lectures**

Enzymatic and Microbial methods in asymmetric synthesis. Use of different types of enzymes lipases, oxidases etc. in organic synthesis.

**1. The Applications of Spectroscopic Techniques in Structure Elucidation 25 lectures**

**Introduction to FT NMR 10 lectures**

$^{13}\text{C}$  NMR, normal and DEPT spectra and their applications in structure elucidation.

Use of  $^1\text{H}$  NOE in analysis of geometry in three, four and five membered rings and double bonds.

**Problems : 15 lectures**

To discuss the problems by using UV- VIS , I.R., Mass and NMR spectral data for the structure elucidation of organic molecules

**CYL416: Physical Chemistry**

**Credit: 3-0-0**

**Course Hrs. 45**

**Statistical Thermodynamics: (20 Hrs)**

The thermodynamic probability of a system, Types of statistics; Maxwell- Boltzmann distribution law, Fermi- Dirac and Bose- Einstein distribution laws and their comparison. Systems of independent particles. The energy of a system: Ensembles; canonical, micro-canonical and grand canonical ensembles. The partition function. Separation of partition functions into translational, rotational, vibrational and electronic partition functions. Relation between partition function thermodynamic functions. Statistical calculation of equilibrium constants. Relation between entropy and thermodynamic probability.

**Chemical Bonding: (25 Hrs)**

Hamiltonian for diatomic molecules, Born oppenheimer approximation, understanding chemical bonding through molecular orbital treatment of  $H_2^+$ , Bonding and antibonding molecular orbitals, Molecular orbital configurations of homonuclear diatomic molecular, molecular electronic terms, the Valence bond and molecular orbital treatment of hydrogen molecule. Comparison of molecular orbital and valence bond treatments. The Hartree Fock method for molecules. The Virial theorem, the Hellman Feynman theorem, the electrostatic theorem. The free electron molecular orbital method, the Huckel m.o method HMO treatment of butadiene, benzene Extended Huckel method.

**Books Suggested:**

1. Quantum Chemistry, Ira N. Levine Prentice Hall.
2. Introduction to Statistical Thermodynamics, T.I. Hill.

### CYL417: Green Chemistry

#### Credit: 3-0-0

Green Chemistry- Concepts and principles, production of chemical waste, problems associated with it and its prevention. Green process metrics. Green Catalysis – heterogeneous, homogeneous, phase transfer, Biocatalysis, and photocatalysis. Green solvents – Supercritical fluids (carbon dioxide and water), water, ionic liquids and fluorous biphasic solvents. Design for efficiency – photochemical reactions, Microwaves, sonochemistry and electrochemical synthesis. Designing Greener processes – Reactors, inherent safer design, process intensification and in-process monitoring. Industrial case studies – greening of acetic acid manufacture, EPDM rubbers, Vitamin C, improvement in Dyeing, polyethene and eco-friendly pesticides, COFIRM, MACH 2 and INTREPID insecticides. Green polymers - Polyaspartic acid.

Concept of atom-economy: Synthesis of ibuprofen, microbes in synthesis of adipic acid and catechol, activators for hydrogen peroxide oxidation processes. Green reactions – Strecker reaction, halide free synthesis of aromatic amines, selective methylation using dimethylcarbonate.

**Textbook and Course Material:** There will be two required textbooks for the course. Also, some of the material will be taken from current literature:

1. Lancaster, M.; *Green Chemistry an Introductory Text*, Royal Society of Chemistry, Cambridge, UK 2002. ISBN 0-85404-620-8.
2. Cann, M.C.; Connelly, M.E. *Real World Cases in Green Chemistry*, American Chemical Society: Washington DC. 2000. ISBN 0-8412-3733-6 (Paperback) (RWCGC). \$16.00

#### Additional Reference Books:

1. Anastas, P. T.; Warner, J. C. *Green Chemistry: Theory and Practice*, Oxford University Press: Oxford 2000. ISBN: 0 19 850698 8 (Paperback)
2. Matlack, A.S., *Introduction to Green Chemistry*, Marcel Dekker, Inc., New York, 2001.
3. Tundro, P.; Anastas, P., *Green Chemistry Challenging Perspectives*, Oxford Press, Oxford, 2000.
4. Anastas, P.T.; Williamson, T.C., *Green Chemistry, Frontiers in Benign Chemical Syntheses and Processes*, Oxford University Press, Oxford, 1998.
5. Anastas, P.T.; Bickart, P.H.; Kirchhoff, M.M., *Designing Safer Polymers*, Wiley Interscience, NY.
6. *Green Chemical Syntheses and Processes*, ACS Symposium Series 767, Anastas, P.T.; Heine, L.G.; Williamson, T.C. (Editors), American Chemical Society, Washington, D.C., 2000.

**CYP411: Inorganic Chemistry Lab**

**Credit: 0-0-3**

1. Preparation of  $\text{Co}(\text{acac})_3$ , its Characterization using NMR, IR, UV-Vis and Analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7, 525)
2. Preparation of  $\text{Co}(\text{acac-NO}_2)_3$ , its Characterization using NMR, IR, UV-Vis and Analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7, 525)
3. Preparation of  $[\text{Fe}(\text{H}_2\text{O})_6][\text{Fe}(\text{N-salicylideneglycinato})_2]_2 \cdot 3\text{H}_2\text{O}$ , its Characterization using IR, UV-Vis, Magnetic Susceptibility and Analysis of Iron. (ref. Inorganica Chimica Acta, 1977, 23, 35).
4. Preparation of  $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$  its Characterization using IR, UV-Vis, Magnetic Susceptibility and Analysis of Nickel and  $\text{NH}_3$ . (ref. Marr and Rockett, 1972).
5. Preparation of  $[\text{Ni}(\text{ethylenediamine})_3]\text{Cl}_2$  its Characterization using IR, UV-Vis, Magnetic Susceptibility and Analysis of Nickel. (ref. Marr and Rockett, 1972, page 270).
6. Preparation of  $[\text{Fe}(\text{NO})(\text{S}_2\text{CN}(\text{Et})_2)_2]$  its Characterization using IR, UV-Vis, Magnetic Susceptibility and Analysis of Fe(II). (ref. Marr and Rockett, 1972, page 262, J. Chem. Soc. 1962, 84, 3404).
7. Preparation of Octahedral and Tetrahedral Complexes of dichlorodipyridylcobalt(II), Differentiate them using IR, UV and Magnetic Properties. Estimate Co(II) from one of them. (ref. Marr and Rockett, 1972, page 375, Inorganic Chemistry, 1966, 5, 615).
8. Preparation of  $\text{VO}(\text{acac})_2$  and its Piperidine Complex, Characterize using IR, UV and Magnetic Moment. Estimate for V(IV). (ref. Marr and Rockett, 1972, 243).
9. Preparation of Diaquotetraacetataocopper(II), Magnetic Susceptibility IR and UV-Vis, Analysis of Copper(II).
10. Preparation of cis-and Trans-potassium Dioxalato Diaquochromate (III). Interpretation of IR, UV and Magnetic Properties. Estimation of Chromium. (ref. Marr and Rockett, 1972, page 386).
11. Preparation of  $\text{HgCo}(\text{NCS})_4$ , its IR and Measure its Magnetic Moment. (ref. Marr and Rockett, 1972, page 365).

M.Sc. Chemistry (Hons. School) Semester – II  
(Under Credit Based Continuous Evaluation Grading System)

12. Preparation of Sodium Tetrathionate, Interpretation of its IR and Analysis using Potassium Iodate. (ref. Marr and Rockett, 1972, page 214).
13. Preparation of Potassium Dithionate, Interpretation of its IR and Analysis Using Potassium Iodate. (ref. Marr and Rockett, 1972, page 214).
14. Preparation of bis(acetylacetonato)copper(II), UV-Vis, and IR, Magnetic Studies, Demonstration of Jahn Teller Effect by Solution Spectral Studies. (ref. Bull. Chem. Soc. Japan, 1965, 29, 852).
15. Preparation of Salicylamide Complexes of Copper(II). IR, UV, magnetic data and analysis of Cu(II). (ref. Indian J. of Chem., 1977, 15A, No. 5, 459; *ibid*, 1971, 9, 1396).
16. To Prepare a Macrocyclic Ligand 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclo tetradeca-4,11-dienedi(hydrogeniodide) and its Complex with Ni(II). Study IR, NMR and UV-Vis of ligand and Complex and Magnetic Properties of Complex. To analyze for Ni and I. (J. Chem. Edu. 1977, 79, 581).
17. Preparation and Resolution of tris(ethylenediamine)cobalt(III). UV-Vis, NMR, IR, Optical Rotation of the Resolved Complexes. (Ref. Marr and Rockett, 1972, page 386).



### **CYL501: Inorganic Chemistry**

**Credits: 3-0-0**

**(45 hrs.)**

#### **1. Inorganic Chemistry of Biological system (5)**

Introduction, energy sources for life, non-photosynthetic processes Essential and trace elements on biological processes, Biological role of alkali and alkaline earth metal ions with special reference of  $\text{Na}^+$ - $\text{K}^+$  Pump. Porphyrins and metalloporphyrins.

#### **2. Biochemistry of metal ions in biological systems (20 Hrs)**

Biochemistry of iron, iron storage and transport, ferritin, transferrin, hemoglobin and myoglobin, structure and function of hemoglobin, physiology of myoglobin and hemoglobin, nature of heme-dioxygen binding in hemoglobin and myoglobin, model systems, cooperativity in hemoglobin, bacterial iron transport, Other iron-porphyrin biomolecules, peroxidases and catalases, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer, respiration and photosynthesis, Z-Scheme, ferridoxins, and rubredoxin. Bluecopper proteins, superoxide dismutase hemocyanines photosynthesis, chlorophyll and photosynthetic reaction center. Biological role of Molybdenum, Tungsten, Vanadium, Chromium and Nickel. .

#### **3. Enzymes (10)**

Introduction, Mononuclear zinc enzymes, carbonic anhydrase, carboxypeptidase, . Structure and function, inhibition and poisoning Vitamin  $\text{B}_{12}$  and  $\text{B}_{12}$  coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, nitrogenases

#### **4. Metals in Medicine and the Environment (10)**

Introduction, Metallotherapeutics with Lithium, Cisplatin: An Anti-Cancer Drug, Metals in the Environment, Toxicology of cadmium, arsenic, mercury, lead and other heavy metals

#### **Books Recommended:**

1. J. E. Huheey, E. A. Keiter and R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edition, Haper Collins.
2. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edition, John Wiley and Sons.
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 5<sup>th</sup> Edition, John Wiley.
4. Ch. Elschenbroich and A. Salzer, Organometallics. A Concise Introduction, Second Edition, VCH.
5. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, 3rd Edition, Oxford University Press.
6. J.A. Cowan, Inorganic Biochemistry, 2nd Edition, Wiley – VCH.
7. G. Wulfsberg, Inorganic Chemistry, University Science Books.

## **Photochemistry and Pericyclic Reactions**

### **CYL502**

**Credits: 3-0-0**

#### **1. Photochemical Reactions (4 Hrs)**

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

#### **2. Determination of Reaction Mechanism (4 Hrs)**

Classification, rate constants and life times of reactive energy states – determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions – photo-dissociation, gas-phase photolysis.

#### **3. Photochemistry of Alkenes : (6 Hrs.)**

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

#### **4. Photochemistry of Carbonyl Compounds : (8 Hrs.)**

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic,  $\beta$ ,  $\gamma$ -unsaturated and  $\alpha,\beta$ -unsaturated compounds, Cyclohexadienones. Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

#### **5. Photochemistry of Aromatic Compounds : (4 Hrs.)**

Isomerisations, additions and substitutions.

#### **6. Miscellaneous Photochemical Reactions : (4 Hrs)**

Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

#### **7. Pericyclic Reaction : (15 Hrs.)**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward --- Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions --- conrotatory and disrotatory motions,  $4n$ ,  $4n+2$  and allyl systems. Cycloaddition --- antarafacial and suprafacial additions,  $4n$  and  $4n+2$  systems,  $2+2$  addition of ketenes, 1,3-dipolar cycloadditions and cheletropic reactions.

Sigmatropic rearrangements – suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and  $\pi$ -sigmatropic rearrangements. Claisen, Cope and  $\pi$ -aze – Cope rearrangement. Fluxional tautomerism. Ene reaction.

**Chemistry of Materials**  
**CYL503**

**Credits: 3-0-0**

**1. Magnetic Materials (Ferrites) : (8 Hrs.)**

Introduction, structure and classification, hard and soft ferrites, synthesis of ferrites by various methods (precursor and combustion method), characterization of ferrites by Mossbauer spectroscopy, significance of hysteresis loop and saturation magnetization in ferrites, magnetic properties of ferrites, applications of ferrites.

**2. Glasses, Ceramics, Composites and Nanomaterials (4 Hrs.)**

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites, Nanocrystalline phase, preparation procedures, special properties, applications.

**3. Thin Films and Langmuir -Blodgett Films (4 Hrs.)**

Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

**4. Liquid Crystals (10 Hrs.)**

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic - nematic transition and clearing temperature - homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

**5. Ionic Conductors ( 6 Hrs.)**

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

**6. Ionic Liquids (8 hrs.):** Introduction, Types and Unique Physico-chemical properties, Polarity and solvation, liquidus range, vapor pressure, thermal stability, toxicity, recycling, applications in biopolymer processing, gas adsorption, and stable carbon nanotubes dispersions.

**7. Fullerenes, Carbon Nanotubes and Graphene (5 hrs):** Types and Properties, Methods of Preparation and separation of carbon nanotubes, applications of fullerenes, CNTs and graphene.

**Books Suggested:**

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D. Callister, Wiley.
3. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.
4. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
5. Handbook of Liquid Crystals, Kelker and Hatz, Chemie Verlag.
6. Ferrite materials by V.R.K. Murthy & B. Viswanathan, Sprniger Verlag, Berlin, 1990.
7. Ionic Liquids in Synthesis, Ed., P. Wasserscheid and T. Welton, 2008.

**Inorganic Chemistry**  
**CYL504**

**Credits: 3-0-0**

1. **Organometallic Chemistry of transition elements** : Isolobal analogies, synthesis, structure and bonding, organometallic reagents in organic synthesis and in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerization); pi-acid metal complexes, activating of small molecules by coordination.

**( 5 Hrs)**

2. (a) Hybridization VSEPR theory, symmetry elements and point groups for simple molecules, determination of point groups, use of symmetry in determining symmetry of molecular orbitals, atomic orbitals and ligand group orbital (LGO),  $\sigma$  bond and  $\pi$  bonding energy level diagrams of octahedral, tetrahedral and square planar complexes.
- (b) Isomerism, octahedral and tetrahedral crystal field splittings of d orbitals, CFSE, magnetism and colour of transition metal ions, LS coupling scheme, correlation diagram of d1 d2 ion in octahedral case. : Coordination chemistry of transition metal ions: stability constants of complexes and their determination; stabilization of unusual oxidation states, stereochemistry of coordination compounds, Ligand field theory, splitting of d-orbitals in low-symmetry environments. Jahn-Teller effect, interpretation of electronic spectra, Orgel diagrams, Tanabe Sugano diagrams, the determination of  $Dq$ ,  $\beta$  using spectroscopic data including charge transfer spectra; spectrochemical series, nephelauxetic series, magnetism; paramagnetism, ferromagnetism and anti-ferromagnetism, quenching of orbital angular moment spin orbit coupling, inorganic reactions, photochemical reaction of chromium and ruthenium complex, fluxional molecules iso- and heteropolyacids; metal clusters, spin crossover in coordination compounds.

**(25 Hrs)**

**3. Inorganic Reaction Mechanisms: (15 Hrs)**

Rate laws and stoichiometric reaction mechanisms for ligand substitution reaction, intimate mechanism for ligand substitution reaction, entering group, leaving group, metal effects on ligand substitution rates, spectator ligand effects on ligand substitution rates, classification of redox reaction mechanism, outer sphere electron transfer processes, one electron inner sphere and long range electron transfer processes, two electron inner sphere electron-transfer processes.

**Books Recommended:**

1. J. E. Huheey, E. A. Keiter and R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4<sup>th</sup> Edition, Haper Collins.
2. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> Edition, John Wiley and Sons.
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 5<sup>th</sup> Edition, John Wiley.
4. Ch. Elschenbroich and A. Salzer Organomettalics, A Concise Introduction, Second Edition, VCH.
5. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, 3<sup>rd</sup> Edition, Oxford University, Press.
6. J.A. Cowan, Inorganic Biochemistry, 2<sup>nd</sup> Edition, Wiley – VCH.
7. G. Wulfsberg, Inorganic Chemistry, University Science Books.

**Bio-organic Chemistry**  
**CYL505**

**Credits: 3-0-0**

**1. Carbohydrates (8 Hrs.)**

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars, N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides – cellulose and chitin. Storage polysaccharides – cellulose and chitin. Storage polysaccharides – starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrate metabolism – Krebs's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

**2. Amino – acids, Peptides and Proteins : (6 Hrs.)**

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures.  $\alpha$ -helix,  $\beta$ -sheets, super secondary structure, triple helix structure of collagen, Tertiary structure of protein – folding and domain structure. Quaternary structure.

Amino – acid metabolism – degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH)

**3. Nucleic Acids : (5 Hrs.)**

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, and overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

**4. Enzymes : (8 Hrs.)**

Introduction and historical perspective, proximity effects and molecular adaptation. Chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

**5. Mechanism of Enzyme Action : (3 Hrs.)**

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

**6. Kinds of Reactions Catalysed by Enzymes : (6 Hrs.)**

Nucleophilic displacement on a phosphorus atom, multiple displacement reaction and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions,  $\beta$ -cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

**7. Co-Enzyme Chemistry : (4 Hrs.)**

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

**8. Enzyme Models : (5 Hrs.)**

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and procirality. Biomimetic chemistry, crown ethers, cryptates. Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes.



**Bio-physical Chemistry****CYL506****Credits: 3-0-0****UNIT-I (23 Hrs)**

**Biological Cell and its Constituents:** Biological Cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition.

**Bioenergetics:** Standard free energy change in biochemical reactions, exergonic, endergonic, Hydrolysis of ATP, synthesis of ATP from ADP, coupled reactions, degree of coupling.

**Statistical Mechanics in Biopolymers:** Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures, introduction to protein folding problem.

**Biopolymer Interactions:** Forces involved in biopolymer interactions, Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curves.

**Thermodynamics of Biopolymer Solutions:** Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.

**Cell Membrane and Transport of Ions:** Structure and functions of cell membrane. Active transport across cell membrane, irreversible thermodynamics treatment of membrane transport.

**UNIT- II (22 hrs.)**

**Bio-Polymers and their Molecular Weights:** Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques.

**Viscosity:** Measurement, relation to geometry and correlation with hydrodynamic properties.

**Diffusion:** Fick's Law of diffusion, diffusion coefficient and its interpretation, frictional coefficient.

**Ultracentrifugation:** Svedberg equation, sedimentation equilibrium, density gradient sedimentation.

M.Sc. Chemistry (Hons. School) Semester – IV  
(Under Credit Based Continuous Evaluation Grading System)

**Electrophoresis:** General principles, Double layer techniques, moving boundary electrophoresis, zonal electrophoresis, isoelectric focusing.

**Osmotic Pressure:** Second virial coefficient, Donnan effect, molecular mass and geometry from O.P. data.

**Optical Properties of Biomacromolecules:** Light Scattering, fundamental concepts, Rayleigh Scattering, Scattering by Larger particles.

**Books Recommended:**

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, Voet and Voet, John Wiley.
4. Macromolecules: Structure and Function, F.Wold., Prentice Hall.
5. Text Book of Polymer Science, F.W. Billmeyer.
6. Physical Chemistry of Polymers, A. Tager.

**(Optional Course)**  
**Organic Chemistry-V**  
**(Advanced Organic Synthesis)**  
**CYL566**

**Credit: 4-0-0**

**1. Newer Synthetic Reactions and Reagents**

**45 Hrs**

**A. Chemistry of Carbanions**

**15 Hrs**

Enolates, Thermodynamic versus Kinetic enolates, enolate equivalents and enamines: Applications in carbon-carbon bond formation and related reactions. Applications in chiral synthesis.

Phosphorus, Sulphur and nitrogen ylides: Preparation, applications in organic synthesis and mechanism.

Umpolung reactions (sulphur compounds, nitro compounds, lithiated ethers and related compounds).

**Phase Transfer Catalysis**

**5 Hrs**

Principles and applications of phase transfer catalysis, crown ethers and polymer- supported reagents in organic synthesis.

**Green Chemistry**

**10 Hrs**

Principles of Green Chemistry and its applications: Biotransformations: Classification of enzymes, advantages and disadvantages, applications in organic synthesis; Principles of ultrasound and microwave assisted organic synthesis. Reactions in ionic liquids

**Organosilicon Compounds:**

**15 Hrs**

Preparation and applications in organic synthesis; Applications of Pd(0) and Pd(II) complexes in organic synthesis- Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi Coupling. Preparation and applications of lithium organocuprates.

**2. Disconnection approach:**

**15 Hrs**

An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

**Books Recommended:**

1. Designing Organic Synthesis, S. Warren, Wiley
2. Organic Synthesis- Concepts, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlag VCH.
3. Advanced Organic Synthesis Part A and B, F.A. Carey and R. J. Sundberg, Plenum Press.
4. Principles of Organic Synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
5. *Modern Methods of Organic Synthesis* Cambridge University Press (1971). Carruthers, W.

**(Optional Course)**  
**Inorganic Chemistry-VII**  
**(Bioinorganic Chemistry)**  
**CYL570**

**Credits: 4-0-0**

**1. Inorganic Chemistry of Enzymes**

**(30 Hrs)**

Introduction, energy sources for life, non-photosynthetic processes, metalloporphyrins, cytochromes, biochemistry of iron, iron storage and transport, ferritin transferring, bacterial iron transport, hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, physiology of myoglobin and hemoglobin, structure and function of hemoglobin. Other iron-prophyrin biomolecules, structure and function of hemoglobin. Other iron-porphyrin biomolecules, peroxidases and catalases, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer, respiration and photosynthesis; ferridoxins, and subredonim carboxypeptidase, carbonic anhydrase, metallothioneins. Blue copper proteins, superoxide dismutase hemocyanines photosynthesis, chlorophyll and photosynthetic reaction center.

**Enzymes:** Structure and function, inhibition and poisoning Vitamin B12 and B12 coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, bio-inorganic chemistry of Mo and W, nitrogenases: other elements V, Cr, Ni (essential and trace elements in biological systems).

**2. Metal Ions in Biological Systems**

**(20 Hrs)**

Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA). Template temperature, stability of DNA.

Role of metal ions in replication and transcription process of nucleic acids.

Biochemistry of dioxygen, bioinorganic chips and biosensors.

Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land.

Metals in the regulation of biochemical events. Transport and storage of metal ions *in vivo*.

Metal complexes as probes of structure and reactivity with metal substitution.

**3. Inorganic Medicinal Chemistry**

**(10 Hrs)**

Fundamentals of Toxicity and Detoxification. Nuclear medicines.

**Books Recommended:**

1. J. E. Huheey, E. A. Keiter and R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4<sup>th</sup> Edition, Haper Collins.
2. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> Edition, John Wiley and Sons.
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 5<sup>th</sup> Edition, John Wiley.
4. Ch. Elschenbroich and A. Salzer, Organometallics. A Concise Introduction, Second Edition, VCH.
5. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, 3<sup>rd</sup> Edition, Oxford University Press.
6. J.A. Cowan, Inorganic Biochemistry, 2<sup>nd</sup> Edition, Wiley – VCH.
7. G. Wulfsberg, Inorganic Chemistry, University Science Books.
8. S.J. Lippard, & J. M. Berg *Principles of Bioinorganic Chemistry* Univ. Science Books (1994).
9. S. J. Lippard, *Progress in Inorganic Chemistry* Vols. 18 and 38, Wiley-Interscience (1991).

**(Optional Course)**  
**CYL571: Inorganic Polymers**

**Credit: 4-0-0**

**(60 hrs.)**

**Inorganic Polymers: Introduction, importance of Inorganic Polymers, Types of Inorganic Polymers. Characterization of Inorganic Polymers:** Molecular Weights, Molecular Weight Distributions, Other Structural Features, Chain Statistics, Solubility Considerations, Crystallinity, Transitions, Spectroscopy, Mechanical Properties. [5]

**Polyphosphazenes:** Introduction, History, Alternative Synthesis Routes to Linear Polymers: Ring-opening polymerization and Condensation polymerizations. Surface Reactions of Polyphosphazenes, Hybrid Systems through: Block, Comb, or Ring-Linked Copolymers, Composites, Organometallic Polyphosphazenes, Small-Molecule Models, Molecular Structure of Linear Polyphosphazenes, Structure–Property Relationships, Applications of Polyphosphazenes, Optical and Photonic Polymers. [15]

**Polysiloxanes and Related Polymers:** Introduction, History, Nomenclature, Preparation and analysis, General Properties, Reactive Homopolymers, Elastomeric Networks, Some New Characterization Techniques Useful for Polysiloxanes, Copolymers and Interpenetrating Networks, Applications of polysiloxane. [10]

**Polysilanes and Related Polymers:** Introduction, History, Synthesis, Chemical Modification of Polysilanes, Physical Properties of Polysilanes, Electronic Properties of Polysilanes, Chromotropism of Polysilanes, Electrical Conductivity and Photoconductivity, Luminescence of Polysilane, Photodegradation of Polysilanes, Cross-Linking, Structural Arrangements in Polysilanes, Technology of Polysilanes [10]

**Ferrocene-Based Polymers, and Additional Phosphorus- and Boron-Containing Polymers:** Ferrocene-Based Polymers, Other Phosphorus-Containing Polymers, Boron-Containing Polymers [10]

**Miscellaneous Inorganic Polymers:** Introduction, Other Silicon-Containing Polymers, Polygermanes, Polymeric Sulfur and Selenium, Other Sulfur-Containing Polymers, Aluminum-Containing Polymers, Tin-Containing Polymers, Arsenic-Containing Polymers, Metal Coordination Polymers [10]

**Books**

1. James E. Mark, Harry R. Allcock, Robert West, Inorganic Polymers, Second Edition, Oxford University Press (2005)
2. P.B. Saxena, Inorganic Polymers, Discovery Publishing House, 2007
3. Roger De Jaeger, Mario Gleria, Inorganic Polymers, Nova Science Publishers, 2007
4. Ronald D. Archer, Inorganic And Organometallic Polymers, John Wiley & Sons, 2001
5. F.A.Cotton & G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edition 1988.
6. J.E. Hukey, E.A. Keiter And R.L. Keiter, Inorganic Chemistry, Principles Of Structure And Reactivity, 4<sup>th</sup> Edition, Harper Collins College Publisher 1993