

# **FACULTY OF SCIENCES**

## **SYLLABUS**

### **FOR**

**M.Sc. Chemistry (CBCEGS)  
(SEMESTER: I - IV)**

**Examinations: 2016-17**



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**GURU NANAK DEV UNIVERSITY  
AMRITSAR**

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

### SCHEME

#### SEMESTER-I

Sr. No.	Course No.	Paper Title	Course hrs	Credit Hrs.
1	CYL451	Molecular Spectroscopy-I	60	4-0-0
2	CYL452	Organic Synthesis-I (Reaction Mechanism – substitution reactions)	45	3-0-0
3	CYL453	Inorganic Chemistry –I (Transition Metal Chemistry)	45	3-0-0
4	CYL454	Physical Chemistry-I	45	3-0-0
5	CYL455	Supramolecular Chemistry	45	3-0-0
6	CYL299	Computer for Chemists	30	2-0-0
Lab Courses				
7	CYP451	Inorganic Chemistry Lab	90	0-0-3
8	CYP452	Physical Chemistry Lab	90	0-0-3
9	CYP299	Computer Lab	60	0-0-2
		<b>Theory 18 credits; Practical 8 credits</b>		

#### SEMESTER-II

Sr. No.	Course No.	Paper Title	Course hrs	Credit Hrs.
1	CYL461	Molecular Spectroscopy-II	60	4-0-0
2	CYL462	Organic Synthesis-II (Reaction Mechanism – Addition, elimination and rearrangement reactions)	45	3-0-0
3	CYL463	Inorganic Chemistry-II (Reaction Mechanism and organometalics)	45	3-0-0
4	CYL464	Physical Chemistry	60	4-0-0
5	CYL465	Bio-organic & Medicinal Chemistry	45	3-0-0
Lab Courses				
6	CYP461	Organic Chemistry	90	0-0-3
7	CYP462	Electroanalytical Chem. Lab	90	0-0-3
		<b>Theory 17 credits; Practical 6 credits</b>		

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**SEMESTER-III:**

S.No.	Course No.	Course Title	Credit
1	CYL551	Physical Chemistry-III (Quantum Chemistry)	3-0-0
2	CYL552	Organic Chemistry-III (Photochemistry and Pericyclic Reactions)	3-0-0
3	CYL553	Inorganic Chemistry-III	3-0-0
4	CYP551	Dissertation	0-0-18
5		Interdisciplinary Course-I	4-0-0
6		Interdisciplinary Course-II	4-0-0

Dissertation to be submitted before Dec 31 of the year. Viva exams will be held in January of next year

**SEMESTER-IV:**

S.No.	Course No.	Course Title	Credits
1	CYL561	Physical Chemistry-IV	3-0-0
2	CYL562	Organic Chemistry-IV (Biosynthesis of Natural Products)	3-0-0
3	CYL563	Inorganic Chemistry-IV (Inorganic materials and nuclear chemistry)	3-0-0
4	CYP561	Organic Chemistry Lab – II Multi-step Synthesis in Organic Compounds	0-0-3
5	CYP562	Inorganic Chemistry Lab - II	0-0-3

**OPTIONAL COURSES**

*Chose any three courses*

6	CYL564	Physical Chemistry-V (Chemistry of Materials)	4-0-0
7	CYL565	Physical Chemistry – VI (Bio-Physical Chemistry)	4-0-0
8	CYL566	Organic Chemistry-V Advanced Organic Synthesis	4-0-0
9	CYL567	Organic Chemistry-VI (Spectroscopy in Structure Elucidation and Asymmetric Synthesis)	4-0-0
10	CYL568	Inorganic Chemistry-V (Inorganic Spectroscopy)	3-0-0
11	CYL570	Inorganic Chemistry-VII (Bioinorganic Chemistry)	4-0-0
12	CYL571	Inorganic Polymers	4-0-0

**Molecular Spectroscopy – I**  
**CYL451**

**Credit 4-0-0**

- 1. General Features of Spectroscopy: (5 Hrs.)**  
Units and conversion factors. Introduction to spectroscopy, Nature of radiation. Energies corresponding to various kinds of radiation, Experimental techniques, intensities of spectral lines, Selection rules and transition moments, Line widths, Broadening.
- 2. Nuclear Magnetic Resonance Spectroscopy: (35 Hrs.)**  
PMR: Natural abundance of  $^{13}\text{C}$ ,  $^{19}\text{F}$  and  $^{31}\text{P}$  nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, proton exchange, spin-spin coupling- splitting theory, one, two and three bond coupling, virtual, long range and allylic coupling, magnitude of coupling constant; factors affecting the coupling constant, Chemical and magnetic equivalence, First and second order spectra,  $A_2$ , AB, AX,  $AB_2$ ,  $AX_2$ ,  $A_2B_2$  and  $A_2X_2$  spin systems, Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents), CW and FT NMR, Relaxation processes, T1 and T2 measurements, Applications of PMR in structural elucidation of simple and complex compounds.  
 $^{13}\text{C}$ -NMR: Resolution and multiplicity of  $^{13}\text{C}$  NMR,  $^1\text{H}$ -decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE and origin of nuclear overhauser effect. off-resonance, proton decoupling, Structural applications of  $^{13}\text{C}$ -NMR., pulse sequences, pulse widths, spins and magnetization vectors, DEPT, INEPT, Introduction to 2D-NMR, COSY, NOESY, HSQC spectra
- 3. Mass Spectra: (10 Hrs.)**  
Introduction, methods of ionization EI & CI, Brief description of LD, FAB, SIMS, FD etc., Ion analysis methods (in brief), isotope abundance, Metastable ions, general rules predicting the fragmentation patterns. Nitrogen rule, determination of molecular ion peak, index of H deficiency, fragmentation patterns for aliphatic compounds, amines, aldehydes, Ketons, esters, amides, nitriles, carboxylic acids ethers, aromatic compounds etc.

**4. UV and Visible Spectroscopy of organic molecules: (10 Hrs.)**

Measurement techniques, Beer – Lambert's Law, molar extinction coefficient, oscillator strength and intensity of the electronic transition, Frank Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra, Chromophores, auxochromes, blue shift, red shift, hypo and hyperchromic effect,  $\sigma\text{-}\sigma^*$ ,  $\pi\text{-}\pi^*$ ,  $n\text{-}\pi^*$  transitions in organic molecules, Woodward rules for conjugated dienes and  $\alpha$ ,  $\beta$ - unsaturated carbonyl groups, extended conjugation and aromatic sterically hindered systems, Quantitative applications.

**Books Recommended:**

1. Pavia, Lampman & Kriz, Introduction to Spectroscopy.
2. C.N Banwell "Fundamentals of Molecular Spectroscopy".
3. R. M. Silverstein, G.C.Bassler, T.C. Morrill, "Spectrometric Identification of Organic Compounds.
4. W. Kemp, "Organic Spectroscopy".
5. D.H. Williams, I. Fleming, "Spectroscopic Methods in Organic Chemistry".
6. D.H. Williams, I. Fleming, "Spectroscopic Problems in Organic Chemistry", 1967.
7. R.C. Banks, E.R. Matjeka, G. Mercer, "Introductory Problems in Spectroscopy", 1980.
8. G.M. Barrow "Introduction to Molecular Spectroscopy".

**Organic Synthesis –1**  
**(Reaction Mechanism-Substitution Reactions)**  
**CYL452**

**Credit 3-0-0**

- 1. Reaction Mechanism: Structure and Reactivity** **12 Hrs**  
Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.
- 2. Aliphatic Nucleophilic Substitutions** **10 Hrs**  
The  $S_N2$ ,  $S_N1$ , missed  $S_N1$  and  $S_N2$  and SET mechanisms.  
The neighbouring group mechanism, neighbouring group participation by  $\pi$  and  $\sigma$  bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The  $S_Ni$  mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. Gabriel synthesis
- 3. Aliphatic Electrophilic Substitutions** **5 Hrs**  
*Bimolecular mechanisms-  $S_E2$  and  $S_{Ei}$ . The  $S_{E1}$  mechanism*, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity, Hell-Volard-Zelinsky reaction ,
- 4. Aromatic Nucleophilic Substitution** **5 Hrs**  
The  $S_NAr$ ,  $S_N1$ , benzyne and  $S_{RN}1$  mechanisms, Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

**5. Aromatic electrophilic substitution**

**7 Hrs**

The arenium ion mechanism, orientation and reactivity in mono substitution and di-substituted aromatics, energy profile diagram, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles. Diazo coupling, Vilsmeier reaction, Gatterman-Koch reaction, Bechmann reaction, Hoesch reaction.

**6. Free Radical Reactions**

**6 Hrs**

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

**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

**Inorganic chemistry-I**  
**(Transition Metal Chemistry)**  
**CYL453**

**Credit : 4-0-0**

**1. Symmetry and Group Theory (10 Hrs)**

Symmetry elements, symmetry Operations symmetry elements commonly occurring molecules like  $\text{NH}_3$ ,  $\text{CH}_4$ ,  $\text{SF}_6$ ,  $\text{PF}_5$ ,  $\text{SF}_4$ ,  $\text{Ni}(\text{CO})_4$ ,  $\text{Fe}(\text{CO})_5$ , determination of point groups, use of character table for determining the reducible and irreducible representation, determination of symmetry of atomic orbitals under different point groups, determination of atomic orbital involved in  $sp$ ,  $sp^2$ ,  $sp^3$ ,  $dsp^2$ ,  $d^2sp^3$  hybridization on basis of group theory and quantitative discussion on concept of hybridization (Text 1 & 2).

**2. Complexes of *f*-Acid Ligands (10 hrs)**

(a)  $\pi$  acceptor character of  $\text{CO}$ ,  $\text{N}_2$ ,  $\text{O}_2$ ,  $\text{NO}$  molecules in terms of MOEL diagrams,  $\pi$  acid ligands of other groups of periodic table. Semi-bridging in metal carbonyls and isocyanides of metals. Magnetic, IR and X-ray diffraction evidence of their structure,  $\pi$  acidity and softness, Symbiosis and antisymbiosis,  $\pi$  complexes of unsaturated organic molecules (bonding with  $\text{C}_2\text{H}_4$  only). (Text 4, suppl. 5, Chap. & Suppl.).

(b) Structures & the IR spectral properties representative transition metal carbonyl complexes.

**3. Chemistry of Transition Metals (25 Hrs.)**

- LS coupling, derivation of spectroscopic terms for  $d^1$  to  $d^9$  electronic configurations, correlation diagram for  $d^2$  ion in octahedral field, splitting of  $d^1$  to  $d^9$  terms in an octahedral and tetrahedral field.
- Selection rules of d-d transitions. Vibronic and spin orbit coupling, effecting of weak to strong cubic fields on R-S terms, Comparison of CFSE values of  $d^1$  to  $d^9$  ions in terms of orbit splitting and R-S term splitting. Effect of CFSE on thermodynamic properties, lattice energy, heat of hydration heat of ligation and spinal structure. Orgel and Tanabe Sugano diagrams, spectra of octahedral, tetrahedral, distorted octahedral (Jahn Teller Effect) and square planar complexes spectrochemical series, nephelauxetic effect, Calculation of  $\beta$  and  $10 Dq$  from spectral data.
- Molecular orbital theory-composition of ligand groups, orbitals, sigma and pi-molecular orbitals MOEL, diagrams of  $\text{Oh}$ ,  $\text{Td}$  and  $\text{D}_{4h}$  complexes with and without pi-bonds, charge transfer spectra.

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- d) Magnetic properties of transition metal ions and free ions presentive, Diamagnets and Paramagnets & ferromagnets. Effects of L-S coupling on magnetic properties. Temperature independent paramagnetism (TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT). Quenching of orbital angular momentum by crystal fields in complexes in terms of term-splitting. Effect of spin-orbit coupling and A, E & T states, Mixing in effect, first order and second order Zeeman effects. Spin-paired and spin-free equilibria in complexes magnetic properties of polynuclear complexes, involving OH, NH<sub>2</sub> and CN bridges. (Texts 3, 7 suppl. 8 : 1).

**Books Recommended:**

1. R.S. Drago, Physical Methods in Inorg. Chem. 1st and 2<sup>nd</sup> Edition, London, 1977.
2. F.A. Cotton, Chemical Application of group theory, 2<sup>nd</sup> Edition.
3. B.N. Figgis, Introduction to Ligand Fields, First Edition.
4. F.A. Cotton & G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edition.
5. F. Basolo and R.C. Johnson, Coordination Chemistry, 1<sup>st</sup> Edition.
6. J.E. Huheey, Inorganic Chemistry, 3<sup>rd</sup> Edition.
7. A.B.P. Lever, Inorganic Electronic-Spectroscopy, 2<sup>nd</sup> Edition.
8. A. Earnshaw, Introduction to Magnetic Chemistry, 1<sup>st</sup> Edition.

**Physical Chemistry – I**  
**CYL454**

**Credit: 3 -0-0**

- 1. Thermodynamics: (15 Hrs)**  
Laws of Thermodynamics, free energy, chemical potential and entropy, Determination of partial molar free energy, volume and heat content, and their significances. Concept of fugacity and determination of fugacity in liquids and gases.

Non ideal systems: Excess functions for non-ideal solutions, Activity, activity Coefficient. Debye Huckel theory for activity coefficient of electrolytic solutions; determinaiton of activity and activity coefficient, ionic strength. The Debye Huckel Theory and its applications. Numerical Problems.

Non Equilibrium Thermodynamics : Thermodynamic criteria for non equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (for example heat flow, chemical reaction, etc.), generalized forces and fluxes, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.
- 2. Statistical Thermodynamics (10 Hrs.)**  
Thermodynamics probability and most probable distribution of a system, Maxwell-Boltzmann distribution law. Ensembles: canonical, grand canonical and micro canonical. Partition functions; translational, rotational, vibrational and electronic. Calculation of thermodynamic properties in terms of partition functions. Application of partition function to calculate heat capacities and equilibrium constants, relation between entropy and thermodynamic probability, Fermi-Dirac and Bose-Einstein statistics. Numerical problems.
- 3. Chemical Dynamics: (20 Hrs)**  
Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation, concept of energy of activation, potential energy surfaces; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions. Lindemann-Christiansen hypothesis, Hinshelwood treatment and Rice Ramsperger-Kassel-Marcus (RRKM) theories of unimolecular reactions. General features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and nuclear magnetic resonance method.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen bromine and hydrogen-chlorine reactions).

**Books Recommended:**

1. Physical Chemistry P.W. Atkins.
2. Thermodynamics for Chemists by S. Glasstone.
3. Chemical kinetics K.J. Laidler.
4. Principles of Physical Chemistry, S.H. Maron & C.F. Prutton.
5. Introduction to the Thermodynamics of Biological Processes by D. Jou & J. E. LLebot.

## **Supramolecular Chemistry**

**CYL455**

**Credit 3-0-0**

**45Hrs.**

**1. Concepts:**

Definition and Development of Supramolecular Chemistry, classification of Supramolecular Host-Guest compounds, Pre- organization and Complementarity, Receptors, Nature of Supramolecular interactions.

**2. Cation Binding Host:**

Crown ethers, Lariat ether and Podands, Cryptands, spherands, selectivity, Macro cyclic, Macrobicyclic and Template effects, soft ligands, calixarenes, carbon donor and - acid ligands, siderophores.

**3. Binding of anions:**

Biological anion receptors, concepts on anion host design, From cation to anion hosts- a simple change in pH, Guanidinium- based receptors, Neutral receptors, organometallic receptors, coordination interactions.

**4. Binding of Neutral Molecules:**

Inorganic solid state clathrate compounds, solid state clathrates of organic hosts, intracavity complexes of neutral molecules, supramolecular chemistry of fullerenes.

**5. Crystal Engineering:**

Concepts, crystal structure prediction, Crystal Engineering with hydrogen bonds, weak hydrogen bonds, hydrogen bonds to metals and metal hydrides, - stacking, coordination polymers.

**6. Molecular Devices:**

Introduction, Supramolecular photochemistry, molecular electronic devices: Switches, wires and rectifiers, machines based on catenanes and rotaxanes.

**Book :**

1. J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York.

**Computer for Chemists**  
**CYL299**

**Credit :2-0-0**

**1. Computer Programming in C Language**

**30 Hrs.**

Principles of programming, algorithms and flowcharts.

Elementary programming, a typical C program, printf function.

Introduction of declarations, assignments and variables: concept of an integer, concept of a variable, rules for naming variables, assignment statement, arithmetic operators.

Integer arithmetic expressions, truncation effects, relative priority of arithmetic operators, use of parenthesis, modulus operator.

Floating point numbers, scientific notation, converting integers to floating point and vice versa , coercion and cast operator, type char.

Decision making in C, scanf function, relational operators, logical operators, if statement, if else statement, nesting of if statement.

p, do while loop, for loop, nesting of for loop.

Type char and ASCII code, character strings and how to print them, octal and hexadecimal notation.

User defined functions, returning value from a function, functions with more than one parameters.

Arrays, declaring an array, initializing an array, break statement, strings and character arrays, sorting an array, finding maximum and minimum in an array, multidimensional arrays.

Input and output.

**Recommenmded Books:**

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.
2. Mullish Cooper, The spirit of c, An Introduction to Modern Programming.

**Inorganic Chemistry Lab**  
**Paper : CYP-451**

**Credit:0-0-3**

**Note:** For each of the preparations, apart from the studies written against each preparation, the student must record information about yield, color, melting point, solubility and drying of the sample, preferably in vacuum.

- 1 Preparation of tris(acetylacetonato)cobalt(III),  $\text{Co}(\text{acac})_3$ , record and interpret its proton and  $^{13}\text{C}$  NMR, IR and UV-vis studies.  
[Ref. J. Chem. Edu. **1980**, 57(7) 525].
- 2 Preparation of tris(nitro-acetylacetonato)cobalt(III),  $\text{Co}(\text{acac-NO}_2)_3$ , record and interpret its proton NMR spectrum.  
[Ref. J. Chem. Edu. **1980**, 57(7) 525].
- 3 Preparation of tris(thiourea)mercury(II), record and interpret its IR and how it helps to establish metal-ligand bonding. .  
[Ref. Inorg. Synth. Vol. VI, p.26].
- 4 Preparation of  $[\text{Fe}(\text{NO})(\text{S}_2\text{CNEt}_2)_2]$ , record and interpret its IR spectrum.  
[Ref. Marr and Rockett, 1972, p. 262].
- 5 Preparation of copper(I) iodide and then prepare the mixed-valent complex,  $[\text{Cu}(\text{en})_2][\text{CuI}_2]_2$ . Record and interpret its UV-vis, magnetic susceptibility.  
[H. Brauer, Handbook of Preparative Chemistry, Vol 2, p 1007; Inorg. Synth. Vol. V 5, p. 16]
- 6 Preparation of [chloro(pyridine)cobaloxime(III)], record and interpret its IR, and UV-vis. spectral data [Inorg. Synth. Vol. XI, p. 61].
- 7 Preparation of  $[\text{Zn}(\text{acac})_2] \cdot \text{H}_2\text{O}$ , record and interpret its IR spectrum TGA/DTA/DSC..  
[Ref. Inorg. Synth. Vol. X, p.74].
- 8 Preparation of polymeric  $\{\text{HgCo}(\text{NCS})\}_n$ , record and interpret its IR, and magnetic susceptibility.  
[Ref. Marr and Rockett, 1972, p. 365].
- 9 Preparation of tris(acetylacetonato)manganese(III),  $\text{Mn}(\text{acac})_3$ , record and interpret its IR, UV-vis and magnetic susceptibility. .  
[Ref. Inorg. Synth. Vol. VII, p.183].
- 10 Preparation of tris(ethylenediamine)nickel(II) dichloride,  $[\text{Ni}(\text{en})_3]\text{Cl}_2$ , record and interpret its IR, UV-vis, magnetic susceptibility. Calculation of Dq and B and values and comparison with hexaaquanickel(II) chloride.  
[Ref. Marr and Rockett, 1972, p. 270].

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- 11 Preparation of  $[\text{VO}(\text{acac})_2]$ , record and interpret its IR, UV-vis and magnetic susceptibility.  
[Ref. Marr and Rockett, 1972, p. 243].
- 12 Preparation of bis(tetraethylammonium)tetrachlorocuprate(II),  $[\text{Et}_4\text{N}]_2[\text{CuCl}_4]$ , record and interpret its UV-vis and magnetic susceptibility. .  
[Ref. Inorg. Synth. Vol. IX, p.141].
- 13 Preparation of lead tetraacetate. [Ref. Inorg. Synth. Vol. I, p.47].
- 14 Prepare a sample of tin(IV) tetraiodide and purify it using rotary evaporator or Soxhlet extractor [Ref. H Brauer, Handbook of Preparative Chemistry, Vol 1, p. 735]

**Physical Chemistry Lab – I**  
**CYP452**

**Credits : 0-0-3**

1. To determine the freezing point depression constant of camphor using naphthalene as solute. Hence determine the molecular weight of acetanilide by Rast's micro method. (J.B. Yadav, page – 36).
2. Determination of molecular weight of a non-volatile substance by measuring elevation of boiling point (Findlay, page – 126).
3. Determination of heat of solution of a substance by solubility method (J.B. Yadav, page – 94).
4. To construct phase diagram of 3-component system ( $\text{CH}_3\text{COOH} + \text{CHCl}_3 + \text{H}_2\text{O}$ ) (J.B.Yadav, page – 131).
5. To prepare and study Hardy – Schulze's rule for arsenious sulphide / Ferric hydroxide sols, (Findlay, page – 402).
6. To determine the relative strength of acids by study kinetics of hydrolysis of an ester (J.B.Yadav, page – 260).
7. To determine the iodine value of given sample of oil (Linseed oil), (Cock & van Rede, page-109).
8. To determine the saponification value of given sample of oil (Ground nut oil), (Cock & van Rede page-117).
9. Determination of interplanar distance of given sample (Sodium Chloride, Urea) by X-ray powdered spectrometer.
10. To obtain the mutual solubility curve of phenol +  $\text{H}_2\text{O}$ , and hence the Upper Consolute point, (J.B. Yadav, page – 109).
11. To determine the coefficient of viscosity of given liquid by Ostwald's viscometer (J.B. Yadav, page – 57).
12. To find the molecular weight of polymer by viscosity measurements, (Findlay, page – 96).
13. Determination of surface tension of given liquid by drop no. method by stalgmometer, (J.B. Yadav, page – 75).
14. To determine the C.M.C. of a soap (sodium or potassium lauryl sulphate by surface tension measurements, (J.B.Yadav, page – 82).
15. To determine the distribution coefficient of  $\text{I}_2$  between  $\text{CCl}_4$  and  $\text{H}_2\text{O}$ , (J.B. Yadav, page – 119).
16. To find the molecular Weight of given liquid by steam distillation method, (J.B. Yadav, page – 107).
17. Determination of transition temperature of given substance by thermometric/ dilatometric method. (J.B.Yadav, page – 82).
18. i) Find water equivalent of Dewar's flask and ii) heat of neutralization of strong acid vs strong base, weak base vs. strong acid using Dewar's flask (Findlay, page 217).

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19. Determination of specific and molar refraction of a liquid by Abbe refractometer. (J.B. Yadav, page – 174).
20. Determine the refraction equivalents of C, H, and Cl atoms. (J.B. Yadav, page – 165).
21. Study and verify the freundlich adsorption isotherm for adsorption of  $\text{CH}_3\text{COOH}$  from its aqueous solution by activated charcoal. (Findlay, page 373).

**Books Recommended:**

1. Findlay's Practical Physical Chemistry.
2. Advanced Practical Physical Chemistry by J.B. Yadav.
3. Laboratory Handbook for Oil & Fat Analysis by L.V. Cock and C. van Rede.

**Computer Lab  
CYP299**

**Credit : 0-0-2**

**Development of Small Computer Codes Involving Simple Formulae in Chemistry:**

1. Calculation of mean, median, mode.
2. Solution of a quadratic equation.
3. Calculation of linear regression.
4. Calculation of curve linear regression.
5. Calculation of Bohr orbit from de Broglie Lambda for electron.
6. Calculation of wave number and frequency from value of wave length.
7. Calculation of van der Waals radii.
8. Radioactive decay.
9. Rate constant of a 1st order reaction, 2nd order reaction.
10. Determination
11. Calculation of lattice energy using Born Lande equation.
12. Addition, multiplication and solution of inverse of 3 X 3 matrix.
13. Calculation of average molecular weight of a polymer containing  $n_1$  molecules of molecular weight  $m_1$ ,  $n_2$  molecules of molecular weight  $M_2$  and so on.
14. Program for calculation of molecular weight of organic compound containing C, H, N, O and S.
15. Calculation of reduced mass of diatomic molecule.
16. Calculate the RMS and most probable velocity of a gas.
17. Calculate the ionic mobility from ionic conductance values.
18. Determine the thermodynamic parameters for isothermal expansion of monoatomic ideal gas.
19. Calculation of value of g- factor from value of J and S.
20. Calculate the bond length and bond angles using crystal structure data.

## Molecular Spectroscopy – II

CYL461

Credit 4-0-0

### 1. Pure Rotational Spectra: (8 Hrs.)

Classification of molecules according to their moment of inertia. Rotational spectra of diatomic molecules (rigid rotator), Intensities of spectral lines, isotopic substitution effects, non-rigid rotator, polyatomic linear and symmetric top molecules, Stark effect.

### 2. Vibrational Spectroscopy (15 hrs)

**Theory of Infrared Absorption:** Harmonic and anharmonic oscillators, absorptions of radiation by molecular vibrations, selection rules, force constant, frequency of vibrational transitions of HCl, vibrations in a polyatomic molecule,  $3N-6$  and  $3N-5$  rules, types of vibrations, overtones, combination and difference bands, examples of  $\text{CO}_2$ ,  $\text{SO}_2$  and  $\text{H}_2\text{O}$ , Fermi resonance, group vibrations.

**Raman Spectroscopy:** Introduction, selection rules, anisotropic polarizability, Stokes, anti-Stokes lines, vibrational Raman spectra of  $\text{CO}_2$  and  $\text{H}_2\text{O}$ , polarised and depolarised Raman Lines, rule of mutual exclusion.

**Determination of IR/Raman Active Modes;** Significance of nomenclature: used to describe various vibrations, use of symmetry considerations to determining the number of active infrared and Raman Lines ( $\text{C}_{2v}$  molecules).

**Applications:** Physical state of a sample, cells used, Application of IR in structure elucidation of organic compounds-carbonyls and effect of substituents on it, C-H, N-H, O-H vibrations and H-bonding- unsaturated, mono- and disubstituted aromatic compounds, metal-ligand vibrations, group frequencies of complex ligands-CN stretching and effect of coordination on it, nitro and nitrite and C=O ligands and effect of their coordination with metal ions.

### 3. Nuclear Quadruple Resonance Spectroscopy: (5 Hrs.)

Introduction, experimental considerations, fundamentals of NQR 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.

### 4. Mössbauer Spectroscopy: (8 Hrs.)

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

**5. Electron Paramagnetic Resonance Spectroscopy: (9 Hrs.)**

Introduction, principle, Presentation of spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, esr spectrum of benzene radical anion, methyl radical.  $\text{CH}_2\text{OH}$  cyclopentadienyl cycloheptatrienyl radical, pyrazine anion, pyrazine anion with  $^{23}\text{Na}$  and  $^{39}\text{K}$  counter ion and 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  $d^5$ , high spin  $d^6$ ,  $d^7$ ,  $d^9$  system). Spectra of triplet states.

**6. X-ray Diffraction Methods of Analysis (9 hrs.)**

Production of X-rays, solid state symmetry, reciprocal lattice, Bragg's law in reciprocal space, the powder method, interpretation of powder pattern of a cubic system, particle size determination by powder method, qualitative and quantitative analysis using powder method. X-ray fluorescence spectroscopy, X-rays emission method, applications (qualitative and quantitative).

**7. Photoelectron Spectroscopy: (6 hrs)**

Introduction, photoelectron spectroscopy, chemical shift, X-ray photoelectron spectroscopy, molecular orbital diagrams of nitrogen and oxygen and their XPS spectra-ESCA, ultraviolet photoelectron spectroscopy (UPS), PES spectrum of nitrogen sample, vibrational structure in the  $\text{N}_2$  UPS spectrum, chemical shifts in XPS, exchange splitting and shake up process

**Books Recommended:**

1. R. S. Drago, "Physical Methods in Chemistry". W.B. Saunders Company.
2. C. N. Banwell "Fundamentals of Molecular Spectroscopy".
3. R. V. Parish, NMR, NQR, EPR & Mossbauer spectroscopy in Inorganic Chemistry. Ellis Horwood, London, 1990.
4. G. M. Barrow "Introduction to Molecular Spectroscopy".
5. E. A. Ebsworth, S. Craddock and D.W. H. Rankin, Structural methods in Inorganic Chemistry, Blackwell Scientific Publications (1991).
6. C.N.R. Rao and J.R. Ferraro, Spectroscopy in Organic Chemistry, Vol. I, Academic Press, 1971.

**Organic Synthesis –II**  
**(Reaction Mechanism- Addition, Elimination and Rearrangement Reactions)**  
**CYL462**

**Credit: 3-0-0**

- 1. Addition to Carbon-carbon and Carbon-Hetero Multiple Bonds: 15 Hrs**  
Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. Addition of Grignard reagents, organozinc, organolithium and Gilman reagents to carbonyl and unsaturated carbonyl compounds. Use of other organometallic reagents in addition reactions. 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 Reactions: 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, DDQ, PCC, CAN, selenium dioxide, peroxyacids, DCC. Oxidation reactions with special emphasis on Baeyer-villiger reaction, Cannizzaro oxidation-reduction reaction,
- 4. Reduction Reactions: 10 Hrs**  
Introduction. Different reductive processes, Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings, Carbonyl compounds – aldehydes, ketones, acids, ester and nitriles. Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis. Sodium borohydride, sodium cyano borohydride, LAH, diisobutyl aluminium hydride, tin hydride, trialkyl tin hydride, trialkyl silanes, alkoxy substituted LAH, DIBAL, diborane, diisooamyl borane, hexyl borane, 9-BBN, isopinocampheyl and diisopinocampheyl borane. Reduction reactions with particular emphasis on Wolf-Kishner reduction, Clemmensen reduction.

**5. Rearrangements:**

**8 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, Shapiro reaction, Fries rearrangement

**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

**Inorganic Chemistry-II**  
**(Reaction Mechanism and organometalics)**

**CYL463**

**Credit: 3-0-0**

**1. Reaction Mechanisms of Transition Metal Complexes (15Hrs.)**

Introduction, ligand replacement reactions, classification of mechanisms, Water exchange rates, formation of complexes from aqueous ions, anation, reaction, aquation and base hydrolysis attack on ligands, reactions, of square planar complexes, mechanism of ligand-displacement reactions; metal carbonyl reactions, reactions of binuclear carbonyls, associative reactions, species with 17 electron, electron transfer processes outer and inner sphere. The Marcus theory, doubly bridged inner-sphere transfer, other electron transfer reactions; two electron transfers, Non-complementary reaction, Ligand exchange via electron exchange, reductions by hydrated electrons, stereochemical non-rigidity, stereochemically non-rigid coordination compounds, Trigonal bipyramidal molecules, systems with coordination number six or more, isomerization and recombinations, tris chelate complexes, metal carbonyl scrambling cluster, rotation within Co shells. (Texts 1 & 4).

**2. Reaction at Coordinated Ligands: (5 Hrs.)**

Hydrolysis of amino acid esters and peptides and amides, Aldol condensation; Imine formation, hydrolysis and substituent exchange. Template effect and macrocyclic ligands (Text 5).

**3. Organometallics: (25Hrs.)**

- I. The basis of 18e<sup>-</sup> Rule, Exceptions to eighteen electron rule.
- II. Preparation of olefin Transition Metal Complexes.
- III. Molecular orbital, Description of bonding of two electron ligands to Transition Metals.
- IV. Preparation of  $\pi$ - enyl complexes, Molecular orbital description of ligands to transition metals.
- V. Dynamic equilibria in allyl complexes.
- VI. Differences between unconjugated & conjugated olefin ligands.
- VII. The bonding of cyclobutadiene to Transition metals.
- VIII. Preparation of cyclobutadiene complexes.

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- IX. Classification, Nomenclature of cyclopentadienyl complexes, Preparation of cyclopentadienyl T. M. Complexes.
- X. Molecular orbital picture of bonding in ferrocene.
- XI. Organic Chemistry of cyclopentadienyl Transition Metal Complexes.
- XII. Preparation of bis  $\pi$  arene complexes, Bonding of Bis-arene complexes.
- XIII. Preparation of cyclopentadienyl complexes.
- XIV. Organometallic Reagents in Organic synthesis.
- XV. Catalysis involving metal complexes intermediates.

**Books Recommended:**

1. F.A. Cotton & G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edition.
2. William W. Porterfield, Inorganic Chemistry, 1<sup>st</sup> Edition.
3. K.F. Purcell and J.C. Kotz, An Introduction to Inorganic Chemistry.
4. M. Tsubutsui, M.N. Levy, A Nakamura & Mori, Introduction to Metal Complex Chemistry, Plenum Press, New York, 1970.
5. C. Elschenbroich and A. Salzer, Organometallics: A concise Introduction, 2<sup>nd</sup> Ed., VCH 1992.
6. J.J. Eisch, The Chemistry of Organometallic Compounds, London, 1967.
7. G.E. Coates, M.L. H. Green and K.W. Wade, Organometallic Compounds, Vol. I, Chapman and Hall.
8. J.E. Huheey, Inorganic Chemistry, 3<sup>rd</sup> Edition.

**Physical Chemistry – II**

**CYL464**

**Credit : 3-0-0**

- a. Solution & Phase Equilibrium (10 Hrs)**  
Solubility and factors affecting solubility, types of solutions, ideal solution, vapour pressure of ideal solutions, boiling point diagrams of binary miscible mixtures and their Distillation diagrams, azeotropes, critical solution temperatures, solubility of gases in liquids, Henry's law, Nernst distribution law, number of extractions, solutions of solids in liquids & chemical equilibrium. Derivation of Gibb's phase rule, phase equilibria of two component systems showing eutectic congruent and incongruent melting points. Triangular method for graphical representation of three component systems; partially miscible three liquid systems. Applications of ternary liquid diagrams; systems composed of two solids and a liquid.
- b. Macromolecule (10 hrs)**  
Types of polymers, regular and irregular polymers, electrically conducting polymers, synthesis of polymers by chain and step reaction polymerization, physical properties of solid polymers (crystallinity, plasticity & elasticity) vulcanization of rubbers, molecular mass determination by osmometry, viscometry, light scattering and ultracentrifuge methods, number and mass average molecular masses, polymer solutions, factors affecting the solubility of polymers.
- c. Adsorption and Surface Phenomena (10 Hrs)**  
Surface phenomena, capillary action, pressure difference across surface (Laplace equation) vapour pressure of droplets (Kelvin equation) physical and chemical adsorption, adsorption isotherms, Derivation of Langmuir, Freundlich, Tempkin and BET adsorption isotherms, Estimation of surface area by BET equation. Heterogeneous catalysis, surface catalyzed unimolecular and bimolecular reactions, Retarded surface reactions, temporary and permanent catalytic poisons, activation energy for surface reactions.
- d. Physical Properties & Molecular Structure (5 Hrs)**  
Molar refraction, polarizability of molecules, dipole moment and its determination, dipole moment and structure of molecules.
- e. Colloidal State (10 Hrs)**  
Classification of colloids, charge and stability of colloidal dispersions, Hardy-Schulze Law, gold number, electrical properties of colloids, electrical double layer and its structure, Stern's theory of double layer, zeta-potential, electrophoresis and electro-osmosis, emulsions and their classification, emulsifiers, gels and their classification, thixotropy. Association colloids; micellar formation, cmc, soap action. Application of colloids.

**Books Suggested:**

1. Principles of physical chemistry, S.H. Maron & C.F. Prutton.
2. Physical Chemistry, K.J. Laidler.
3. Physical Chemistry, P.W. Atkins.
4. Physical Chemistry of Polymers, A. Tager.
5. Text book of Polymers science, F.W. Billmeyer.
6. Heterogenous Catalysis, S.J. Thomson & G Webb.
7. Kinetics and Mechanism, A.A. Frost & R.G. Pearson.

**Bioorganic and Medicinal Chemistry**  
**Paper : CYL465**

**Credit: 3-0-0**

- 1. Enzymes** **8 Hrs**  
Basic considerations. Proximity effects and molecular adaptation. Introduction and historical prospective, 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 labelling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-menten and Lineweaver-Burk plots, reversible and irreversible inhibition.
- 2. Mechanism of Enzyme Action** **5Hrs**  
Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonucleases, lysozyme and carboxypeptidase A.
- 3. Kinds of Reaction Catalysed by Enzymes** **8Hrs**  
Nucleophilic displacement on a phosphorus atom, multiple displacement reaction and the coupling of ATP cleavage to endergonic processes. Transfer of sulphates, addition and elimination reactions, enolic intermediates in isomerization reactions, -cleavage and condensation, some isomerisation and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.
- 4. Co-Enzyme Chemistry** **6Hrs**  
Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, LIPOIC ACID, vitamin B<sub>12</sub>. Mechanisms of reactions catalysed by the above cofactors.
- 5. Drug Design** **18Hrs**  
Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptors interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials.  
LD-50, ED-50 (Mathematical equations excluded)

**Books Recommended:**

1. Principles of Biochemistry By Lehninger
2. Principles of Biochemistry By Voet and Voet
3. The organic chemistry of drug design and drug action By R. B. Silverman, 2<sup>nd</sup> Ed.,  
2004, Academic press
4. An introduction to drug design by S. S. Pandeya and J.R. Dimmock, New Age  
International

**Organic Chemistry Lab**  
**Paper: CYP461**

**Credit: 0-0-3**

**Hrs. 90**

S. No.	Experiment	Chemicals required	Apparatus	Reference
1	Prepare a sample of Ibuprofen and record its $^1\text{H}$ , $^{13}\text{C}$ NMR spectra			
2	Preparation of oil of Wintergreen from commercial aspirin tablets	Aspirin, methanol, sulphuric acid	Rbf, reflux condenser / microwave oven	<i>J. Chem Edu.</i> , <b>2009</b> , 86, p475
3	Nitration of o-chlorobenzoic acid and o-chloroacetanilide – separation and identification of isomers	o-chlorobenzoic acid, o-chloroacetanilide, nitric acid, sulphuric acid, toluene, ethanol	Rbf, reflux condenser, reaction hood, gloves,	<i>J. Chem Edu.</i> , <b>2008</b> , 85, p1541
4	Preparation of bromohydrin of -methylstyrene	Methyl styrene, NBS, acetone	Rbf, stirrer	<i>J. Chem Edu.</i> , <b>2008</b> , 85, p102
5	Dihydroxylation of cyclohexene with peracids and $\text{KMnO}_4$ – Product distribution by TLC	cyclohexene, oxone, $\text{KMnO}_4$	Rbf, stirrer, TLC,	<i>J. Chem Edu.</i> , <b>2008</b> , 85, p959
6	Preparation of carbene complex of Silver(I) Chloride	2,4,6-trimethylaniline, 40% glyoxal in water, ethanol, p-formaldehyde, toluene, HCl, dioxane, silver(I)oxide, dichloromethane	Rbf, stirrer, reflux condenser, filtration, rotavapor	<i>J. Chem Edu.</i> , <b>2008</b> , 85, p416

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7	Solvent free Cannizaro reaction using p-nitrobenzaldehyde	p-nitrobenzaldehyde, KOH, ethanol	Rbf, reflux condenser	
8	Synthesis of 1,1-diphenylethanol from phenyl magnesium bromide and acetophenone	Bromobenzene, Mg, anhydrous ether, acetophenone, amm. chloride	Two necked Rbf, condenser, dropping funnel, separatory funnel, drying tube,	<i>Modern projects and experiments in organic chemistry</i> By Jerry R. Mohrig, Christina N. Hammond, Paul, F. Schultz, Terence, C. Morill, 2 <sup>nd</sup> Ed, <b>2003</b> , p124
9	Reduction of 3-nitroacetophenone using i) NaBH <sub>4</sub> ii) using Sn and HCl. Identification of the products with NMR, UV, IR spectra	3-Nitroacetophenone, Sn, HCl, absolute ethanol, sodium hydroxide, sodium borohydride	Rbf, stirrer, water bath, centrifuge tube, filtration flask, Buchner funnel	<i>Modern projects and experiments in organic chemistry</i> . P193
10	Synthesis of N,N-diethyl-m-toluamide (mosquito repellent) from m-toluic acid	m-Toluic acid, thionyl chloride, anhydrous ether, diethyl amine	Two necked Rbf, dropping funnel, condenser, adapter, separatory funnel	<i>Modern projects and experiments in organic chemistry</i> . P 227
11	Synthesis of Aspirin, its mode of action and molecular modeling with cyclooxygenase	Salicylic acid, acetic anhydride	Rbf, filtration flask, Buchner funnel,	<i>Modern projects and experiments in organic chemistry</i> . P 29
12	Isolation of essential oils from Caraway seeds and orange peels – (S) – Carvone and (R) - Limonene	Caraway seeds (Shah Jeera)	Pestle mortar, Rbf, steam distillation apparatus, heating mantle/sand bath, separatory funnel	<i>Modern projects and experiments in organic chemistry</i> . P 40

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13	Synthesis of styrene epoxide and ring opening reactions under neutral and acidic conditions	Styrene, <i>m</i> -CPBA,	Rbf, stirrer, suction filtration	
14	Introduction to chemical informatics			<a href="http://www.ch.ic.ac.uk/local/organic/3.html">http://www.ch.ic.ac.uk/local/organic/3.html</a>
15	Molecular modeling – Reactivity of Diels-Alder reaction; Hydrogenation of cyclopentadiene dimer	Software – Gaussian		
16	Diels – Alder reaction of a Danishefsky diene	Trans-4-methoxybutene-2-one, zinc chloride, triethyl amine, trimethyl silyl chloride, maleic anhydride/methyl vinyl ketone	Rbf, Buchner funnel, filtration flask	<i>J. Am. Chem. Soc.</i> , 1974, 96, 7807
17	Synthesis and oxidation of 1-aminobenzotriazole – Benzyne trapping	<i>o</i> -nitroaniline, diethyl malonate, sodium nitrite, sodium acetate, Pd-C (10%), lead tetra-acetate,	Hydrogenator, Rbf, Buchner funnel, filtration flask,	<i>J. Chem. Soc. (C)</i> , 1969, 742

**Electroanalytical Chemistry Lab**  
**Paper: CYP462**

**Credits: 0-0-3**

**A. Conductometry**

1. Find graphically the equivalent conductance at infinite dilution of weak acid (benzoic acid, succinic acid, acetic acid) and hence determine the thermodynamic dissociation constant of the weak acid.
2. Determine the equivalent conductance of strong electrolytes ( $\text{KNO}_3$ ,  $\text{KCl}$ ) at several concentrations of its aqueous solution and verify the Onsager's equation.
3. Determine the equivalent conductance at infinite dilution of weak electrolytes ( $\text{CH}_3\text{COOH}$ ,  $\text{NH}_4\text{OH}$ ) in their aqueous solutions using Kohlraush law.
4. To determine relative strength of monochloroacetic and acetic acid by conductance measurements.

**B. Potentiometry and pHmetry**

5. To determine the dissociation constant of a dibasic acid( malonic acid)
6. The potentiometric titration of a mixture of Chloride and Iodide with  $\text{AgNO}_3$ .
7. To determine the degree of hydrolysis of aniline hydrochloride and hence hydrolysis constant of the salt.
8. Determination of acid and basic dissociation constants of an amino acid and hence the iso- electric point of the acid .
9. Titration of Phosphoric acid solution with  $\text{NaOH}$  using quinhydrone electrode.
10. The Potentiometric Determination of Solute Species in a Phosphate Mixture
11. The Potentiometric Titration of Copper with EDTA.

**C. Electrogravimetry and Coulometric Titrations**

12. Determination of Copper and Lead in a given sample of Brass Electrogravimetrically .
13. Determine coulometrically the concentration of Nickel and Cobalt from a given mixture.
14. The coulometric titration of cyclohexene.

**D. Polarography and Stripping methods**

15. The polarographic Determination of Copper and Zinc in the given sample of Brass.
16. Study the polarographic waves produced by dissolved oxygen.
17. Determine the half wave potential of  $\text{Cd}^{2+}$ , and  $\text{Zn}^{2+}$ , ions in 0.1 M  $\text{KCl}$  solution.
18. Plot a polarogram for a mixture of  $\text{Cd}^{2+}$ ,  $\text{Zn}^{2+}$ , and  $\text{Mn}^{2+}$ , ions.

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19. Determine of formula and the stability constant of complex formation of a metal ion complex.
20. Determine the amount of Copper and Zinc in tap water using DPP.
21. Apply stripping methods to determine the concentration of lead in tap water.

**Amperometric titrations:**

22. Amperometric titration of lead solution with potassium dichromate.
23. Amperometric titration of potassium sulphate solution with Lead nitrate solution.
24. Amperometric titration of nickel in solution with dimethyl glyoxime.
25. Determine transport number of silver and nitrate ions by Hittorf's method.

**Physical Chemistry – III**  
**Quantum Chemistry**  
**CYL - 551**

**Credits : 3-0-0**

**1. Mathematical Preparation (10 Hrs):**

Matrices, square, diagonal unit, scalar, symmetric, hermitian matrices, operations on matrices, determinants, adjoint and inverse of matrix. Use of Cayley Hamilton theorem to find inverse of a matrix, even and odd functions, well behaved functions. Operators and observables, normality and orthogonality of functions, Hermitian operators. Introduction to differentiation and Integration.

**2. Quantum Theory: Introduction and principles and applications (17 Hrs):**

Black Body radiation, planck's radiation law, photoelectric effect, Compton effect, De-Broglie hypothesis, the Heisenberg's uncertainty principle, Rydberg's relation for explaining atomic spectrum of hydrogen. Bohr theory and its limitations. Solution of classical wave equation by separation of variable method, eigen value equation, Hamiltonian operator. Interpretation of  $\psi$ , Solution of particle in one, two and three dimensional box, degeneracy. Postulates of quantum mechanics, the linear harmonic oscillator, and the rigid rotator, quantization of vibrational and rotational energies.

**3. Angular Momentum (6 Hrs):**

Commutative laws, need of polar coordinates, transformation of cartesian coordinates into polar coordinates. Angular momentum of one particle system, orbital angular momentum, the ladder operator method for angular momentum.

**4. The Hydrogen Atom (4 Hrs):**

Outline of various steps in the solution of the electronic Schrödinger equation for hydrogen atom, Radial and angular parts of the hydrogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals. Significance of Quantum numbers, orbital angular momentum and quantum numbers  $m_l$  and  $m_s$ .

**5. The Approximation Methods (5 Hrs.)**

Need for approximation methods, Perturbation and Variation methods and their application to Helium atom.

**6. Chemical Bonding: (3 Hrs)**

Chemical bonding, linear combination of atomic orbitals, overlap integral, coulomb integral, molecular orbital treatment of  $H_2^+$ , Bonding and antibonding orbital of  $H_2^+$

**Books Suggested:**

1. Physical Chemistry, A Molecular Approach by D. A. Macquarrie and J. D. Simon.
2. Quantum Chemistry, Ira N. Levine.
3. Quantum Chemistry, H. Eyring J. Walter and G. E. Kimball. Molecular
4. Quantum Mechanics, P. W. Atkins.

**Organic Chemistry-III**  
**(Photochemistry and Pericyclic Reactions)**  
**CYL552**

**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-dienes,

**4. Photochemistry of Carbonyl Compounds 6 Hrs**

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic,  $\alpha,\beta$ -unsaturated and  $\alpha,\gamma,\delta$ -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 20 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.

**8. Sigmatropic Rearrangements** – suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and  $\sigma$  – sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

**Books:**

1. Fundamental of PhotoChemistry By K.K. Rohtagi Mukherji
2. Molecular Photochemistry By N.J. Turro and W.A. Benjamin
3. Introductory Photochemistry By A. Cox and T. Camp
4. Modern Organic Photochemistry By W. H. Horsepool

**Inorganic Chemistry - III**  
**CYL-553**

**Credits : 3-0-0**

**1. Inorganic chains, rings and cages (15 Hrs.):**

- a) **Chains:** Catenation, heterocatenation, isopolyanions and heteropolyanions.
- b) **Rings:** Borazines, phosphazenes, other heterocyclic inorganic ring systems, homocyclic inorganic systems.
- c). **Cages:** Cage compounds having phosphours, oxygen, nitrogen and sulphur: boron cage compounds, Boranes, carboranes and metallocene carboranes. **(text 1)**

**2. Transition metal cluster compounds ( 15 Hrs.):**

- a) Introduction, metal carbonyl clusters; Low Nuclearity (M3 M4) clusters: isoelectronic and isolobal relationships high nuclearity carbonyl clusters; hetero atoms in metal atom clusters, electron counting schemes for HNCC: HNCC of Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt.
- b) Lower halide and chalcogenide clusters, octahedral metal halide, chalcogenide clusters, triangular clusters, solid state extended arrays.
- c) Compounds with M-M multiple bonds; I) Major structural types; quadrupole bonds, other bond orders in the tetragonal context, relation of clusters to multiple bonds, one dimensional solids, (Text 2, Chap. 23).

**3. Inorganic Chemistry in Biological Systems (15 Hrs.) :**

Porphyrin rings, metalloporphyrins, photosynthesis and respiration, chlorophyll, structure, function and synthetic model Cytochromes; structure and function, CN and CO poisoning, Farredoxins and rubberdoxins, bioredox agents and mechanism, Heamoglobin and myoglobin, structure and mechanism of function, Coperativity, Enzymes, Vitamin B12, B12 Coenzymes; structures and funciton, synthetic model of enzyme action, inhibition on poisoning by ligands and metal ions xanthine oxidase, N2 fixation. **(Text 1 & 2)**

**Books Recommended:**

- 1. J.E.Huheey, Inorganic Chemistry, 3rd Edition, London, 1983.
- 2. F.A. Cotton, I.G. Wilkinson, Advanced Inorganic Chemistry, 5th Edition, New York, 1988.
- 3. D.F. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chem., ELMS, Oxford, 1990

**Physical Chemistry-IV**  
**CYL-561**

**Credit : 3-0-0**

**a) Liquid State: (10 Hrs)**

Introduction to liquid state, thermodynamic properties of liquids, vapour pressure and its determination, enthalpy and entropy of vaporization, Trouton's rule. Intermolecular forces, models and theories of liquids, surface and transport properties, surface tension and its measurement, viscosity and its measurement. Liquid crystals, smectic, nematic and cholesteric mesophases.

**b) Solid State: (10 Hrs)**

Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, Schottky and Frenkel defects, colour centres, non-stoichiometry and defects, solid state reactions. Metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doping semiconductors, superconductors, magnetic materials (ferrites) and their classification.

**c) . Electrochemistry of Solutions (15 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, dielectric constant of liquids containing associated dipoles, ion – solvent nonelectrolyte interactions, change in solubility of non-electrolyte due to primary and secondary solvations.

**d). Photochemistry (10 Hrs.)**

Difference between thermal photochemical reactions, laws of photochemistry, Jablonski diagram, qualitative description of fluorescence, phosphorescence, non-radiative processes (IC, ISC), quantum yield, photosensitized reactions, nuclear geometries of electronically excited states, energy surface description of molecular photochemistry, Excimers and Exciplexes, kinetics of photochemical reactions, chemiluminescence, solar energy conversion and storage.

**Books Suggested:**

1. Principles of Physical Chemistry, S.H. Maron & C.F. Prutton.
2. Solid State Chemistry, C.N.R. Rao.
3. Principles of Solid State Chemistry, P.P. Budnikov & A.M. Ginstling.
4. Physical Chemistry, P.W. Atkins.
5. Modern molecular photochemistry, N.J Turro.
6. Fundamentals of Photochemistry, K.K.Rohtagi- Mukherjee.
7. Applications of Liquid Crystals, G.Meier, E. Sackmann & J.G. Grabmaier.

**Organic Chemistry IV**  
**(Biosynthesis of Natural Products)**  
**CYL – 562**

**Credits : 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.
2. **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:** (26 Hrs)
  - (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:** (5Hrs)  
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. Torssell, 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.

**CYL – 563: Inorganic Chemistry IV**  
**(Inorganic materials and nuclear chemistry)**

**Credits : 3-0-0**

**(45hrs.)**

**A. Inorganic Materials (25 hrs)**

Introduction to the solid state, types of bonding in solids: Ionic, covalent and Metallic bond (bond model). Defects in solids: Point defects, Line defects, Surface defects and Volume defects. p-type and n-type Inorganic semiconductors. Superconductors with special emphasis on synthesis and structure of high temperature superconductors. Properties of inorganic materials: electrical, optical, magnetic and thermal properties.

Nanomaterials: Introduction, classification and importance of nanomaterials. The characteristic differences between nanomaterials and their respective bulk materials. Preparation of nanomaterials: Vapor – phase synthesis, Liquid phase synthesis, Solid – state phase synthesis and other methods. Basic principles of electron microscopy, dynamic light scattering, Atomic force Microscopy and characterization of nanomaterials.

**B. Nuclear and Radiochemistry (20 hrs)**

Radioactive elements, nuclear structure and nuclear stability, binding energy and stability of nuclei, nuclear models. Nuclear reactions: fission and fusion reactions, the interaction of nuclear radiations with matter, Q-value, nuclear reactors (Nuclear fission and fusion reactors). Radioactivity, types of radioactivity, units of radioactivity, Radiation hazards, therapeutics, detectors and their principles. Disintegration constant. Radioactive tracer technique and their applications (in medical, agriculture and industry). Rock and carbon dating.

**Books:**

1. B.C. Harvey, Introduction to Nuclear Chemistry, Prentice-Hall (1969)
2. G. Friedlander, J.W. Kennedy, E.S. Marcus & J.M. Miller Nuclear & Radiochemistry. John-Wiley & Sons (1981)
3. H.V. Keer, Principles of the Solid State, Wiley Eastern Ltd. (1993)
4. A.R. West Solid State Chemistry and Its Applications” John Wiley & Sons (1987)
5. A.K. Cheetham and P. Day Eds. Solid State Chemistry Techniques, Clarendon Press, Oxford (1987)
6. G. Timp Ed. Nanotechnology Springer-verlag (1999)
7. Lesley E. Smart Elaine A.Moor, Solid State Chemistry- An Introduction, 3<sup>rd</sup> edition, Taylor & Francis (2005).

**Organic Chemistry Lab - II**  
**Multi-step Synthesis of Organic Compounds**  
**CYP561**

**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.**

<b>S.No.</b>	<b>EXPERIMENT</b>
<b>1</b>	Synthesize (a) 2,4-dinitro-1-chlorobenzene from chlorobenzene, (b) mixture of <i>o</i> - and <i>p</i> -nitrophenols from phenol and (c) <i>p</i> -nitroacetanilide from acetanilide and make comparison of the reactivity of various substrates and reaction conditions used for performing nitration in each experiment. (Book 2, pp 978-979, 919-20)
<b>2</b>	Synthesis of 2-chloro-4-bromo-6-iodoaniline from aniline.(Book 1, pp 292-299)
<b>3</b>	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)
<b>4</b>	The epoxidation of benzalacetophenone to its epoxide and study its reactivity towards hydroxyl ion. (Book 3, pp 363-364).
<b>5</b>	Michael addition of aniline to benzalacetophenone. (Book 1, p 247)
<b>6</b>	Conversion of benzalacetophenone to its oxime and its transformation to amide and oxazole derivatives. (Book 1, pp 242-247, Book 3 pp 361-365)
<b>7</b>	Synthesis of anthranilic acid from phthalimide. (Book 2, pp 898-899)
<b>8</b>	Synthesis of <i>p</i> -aminobenzenesulfonamide. (Book 1, pp 275-289)
<b>9</b>	Synthesis of Methyl <i>n</i> -pentyl ketone from ethyl acetoacetate. (Book 2, pp 620-621)
<b>10</b>	Synthesis of triphenylcarbinol from bromobenzene. (Book 2, pp 540-541)

**Books:**

- 1.** An Introduction to Modern Experimental Organic Chemistry, R.M. Roberts,., Gilbert, L.B. Rodewald and A.S. Wingrove. Holt, Ranehart and Winston Inc., J.C New York.1969.
- 2.** Vogel's Text Book of Practical Organic Chemistry, 5th Edition.
- 3.** Laboratory Experiments in Organic Chemistry, R. Adams, J.R. Johnson and C.F. Wilcox, The Macmilan Limited, London, 1970.

**Inorganic Chemistry Lab-II**  
**CYP562**

**Credits: 0-0-3**

**S.No.**

**EXPERIMENT**

- 1** Preparation of mercury tetraisothiocyanatocobalt(II). Determination of its magnetic moment and interpretation of its IR spectrum.
- 2** Preparation of nitro-and nitrito-pentaamminecobalt(II) chlorides from chloropenta amine cobalt(III) chloride. Recording and interpreting their electronic and IR spectra.
- 3** Heating the nitro and nitrito isomers at serial 2 to 150 C in an oven for 3 h and recording the infrared spectra again and compare them with the spectra recorded before the isomers were heated.
- 4** Preparation and resolution of tris(ethylenediamine)cobalt(II) ion. Measurement of optical rotation of these resolved complexes.
- 5** Preparation of diaquotetraacetatedicopper(II). Determination of its magnetic susceptibility and interpretation of E.P.R., electronic absorption and IR spectra.
- 6** Preparation of bis(2,4-pentanedione)vanadium(IV) acetate and its piperidine or pyridine complex. Study of both the complexes with the help of infrared, UV-vis spectroscopy and magnetic susceptibility.
- 7** Preparation of hexaamminenickel(II) chloride and tris(ethylenediamine)nickel(II) chloride. Interpretation of their electronic absorption spectral data and calculation of  $\mu_{\text{eff}}$  and  $10Dq$  values. Measurement of magnetic susceptibility, calculation and interpretation of the values.
- 8** Preparation of lead tetraacetate.
- 9** Preparation of potassium trioxalatoaluminate(III) trihydrate. Its TGA and DTA studies and its interpretation of its i.r. data.
- 10** Preparation of disulphur dichloride
- 11** Preparation of sodium tetrathionate, potassium dithionate, and interpretation of their IR spectra.
- 12** Preparation of cis-and trans-potassium dioxalatodiaquochromate(III). Interpretation of their i.r., and electronic absorption spectral data. Calculation of  $\mu_{\text{eff}}$  and  $10Dq$  values.
- 13** Preparation of iron(II) oxalate and potassium trioxalateferrate(III). Interpretation of their magnetic data, E.p.r. and Mossbauer spectra.
- 14** Preparation of nitrosylbis(diethyldithiocarbamate)iron(II) and interpretation of its IR and EPR spectra.

M.Sc. Chemistry (Semester-IV)  
(Under Credit Based Continuous Evaluation Grading System)

- 15** Preparation of chromium(II) acetate hydrate.
- 16** Preparation of 42anganese(II) phthalocyanine. Interpretation of its IR, and electronic absorption spectra.

**Books:**

- 1** G. Marr and B.W. Rockett: Practical Inorganic Chemistry, Van Nostrand Reinhold Company
- 2** W.L. Jolly, The Synthesis and Characterization of Inorganic Compounds. Prentice Hall.

**Optional Courses; Any three to be chosen.**  
**Optional Course**

**Physical Chemistry-V**  
**(Chemistry of Materials)**  
**CYL564**

**Credits 4-0-0**

**1. Multiphase Materials: (8 Hrs)**

Ferrous alloys; Fe-C phase transformation in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

**2. Glasses, Ceramics, Composites and Nanomaterials (10 Hrs)**

Glassy state, glass formers, and glass modifiers, application. Ceramic structures, mechanical properties, clay particle product. Refractories, characterization, properties, and applications. Microscopic composites; dispersion-strengthened and particle reinforced, fibre-reinforced composite, macroscopic composites. Nanocrystalline phase, preparation procedure, special properties, applications.

**3. Thin Films and Langmuir- Blodgett Films (7 Hrs)**

Preparation techniques; evaporation/sputtering, chemical process, sol gel etc. Langmuir – Blodgett (LB) films, growth technique, photolithography, properties and applications of thin and LB films.

**4. Liquid Crystals (12 Hrs)**

Mesomorphic behaviour, thermotropic liquid crystal, 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 crystal. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

**5. High T<sub>c</sub> Materials (12 Hrs)**

Defect perovskites, high T<sub>c</sub> superconductivity in Cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetime, microwave absorption-pairing and multigap structure in high T<sub>c</sub> materials, applications of high T<sub>c</sub> materials.

**6. Materials for Solid State Devices****(5 Hrs)**

Rectifiers, transistors, capacitors –IV-V compounds, low-dimensional quantum structure; optical properties.

**7. Organic Solid, Fullerenes, Molecular Devices****(6 Hrs)**

Conduction organics, organics, organic superconductors, magnetism in organic materials.

Fullerenes- doped, fullerenes as superconductors.

Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory, switches and sensors.

Nonlinear optical materials: nonlinear optical effects, second and third order – molecular hyperpolarisability and second order electric susceptibility – materials for second and third harmonic generation.

**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, Willey.
3. Principle of the Solid State, H.V. Keer, Willey Eastern.
4. Material Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Willey.

**Optional Course**  
**Physical Chemistry-VI**  
**(Bio-physical Chemistry)**  
**CYL565**

**Credits : 4-0-0**

**Fundamentals of Biological Macromolecules**

(25 Hrs)

**Biological Cell and its Constituents:** Prokaryotic and Eukaryotic Cell, Structure and Functions of Ribosomes, Mitochondria, Golgi Apparatus and Cell membrane, and Transport Across Cell Membrane.

**Molecular Basis of life:** Structure of D-glucose & D-fructose; formation of glucosides & the cyclic structure of D-glucose; D-ribose & D-deoxyribose; Structure and conformation of disaccharides and polysaccharides-cellulose, amylose, amylopectin and, Chitin.

**Proteins and Enzymes:** Structure (Primary, Secondary and Tertiary) and Functions of Proteins, Nomenclature, Classification, Enzyme catalysis and its mechanism, Michaelis-Menten Equation, and Lineweaver-Burk equation, Enzyme Activity and Transition State.

**Genetic Material:** Nucleic bases-Types and Structure, Structure and Functions of DNA and RNA.

**Lipids:** Major classes of lipids- Fats & oils; phospholipids, lipoproteins, fatty acids, Structure, classification & role of vitamins & hormones.

**Thermodynamics and Biopolymer Interactions**

(20 Hrs)

**Thermodynamics of Biological Systems:** Basic Concepts, Thermodynamics of Protein Denaturation, Thermodynamic Parameters and Biological events, Standard free energy change in biochemical reactions and effect of pH and concentration, exergonic and endergonic reactions, coupled reactions and their utilization, characteristics of high energy molecules, Synthesis, Structure, Function, and Hydrolysis of ATP, Effect of pH, metal ions and concentration on hydrolysis of ATP.

**Biopolymer Interactions:** Forces involved in biopolymer interactions, Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions, interactions with surfactants and characterization.

**Physical Characterization of Biological macromolecules**

(15 Hrs)

**Optical Properties of Biomacromolecules:** Light Scattering, fundamental concepts, Rayleigh Scattering, Scattering by Larger particles, Information about size and molecular weight.

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

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

M.Sc. Chemistry (Semester-IV)  
(Under Credit Based Continuous Evaluation Grading System)

**Osmotic Pressure:** Second virial coefficient, Donnan effect, molecular mass and geometry from osmotic pressure measurements.

**Isothermal Titration calorimetry:** Basic concept, Application to Protein-Protein, Protein-Ligand, Protein-Drug and Protein Surfactant Interactions.

**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. Biophysical Chemistry, J. P. Allen, 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**

**Spectroscopy in Structure Elucidation and  
Asymmetric Synthesis  
CYL567**

**Credit 4-0-0**

**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.

**2. Organocatalysis in Organic Synthesis (15 Hrs)**

Introduction. Enamine catalysis: Aldol and Mannich type reactions, -heteroatom functionalization, direct conjugate additions via enamine activation. Iminium catalysis: the catalysis concept, cycloaddition reactions, 1,4-addition reactions, transfer hydrogen, cascade reactions. Ammonium ions as chiral templates: Homogeneous catalysis with chiral quaternary ammonium salts, Heterogeneous catalysis- chiral phase transfer catalysis. Morita-Baylis-Hillman reaction: addition of ketones and aldehydes to activated olefins, asymmetric MBH reactions. Asymmetric proton catalysis: conjugate addition reactions, hydrocyanation reactions, mannich reactions, aza-henry reaction, acyl Pictet-Spengler reaction, aza Friedel-Crafts reaction. Chiral Lewis bases as catalysts: allylation reactions, propargylation reactions, hydrocyanation and isonitrile addition, aldol type reactions, reduction of imines, epoxide ring opening. Asymmetric acyl transfer reactions. Nucleophilic N-Heterocyclic carbenes. Ylide based reactions. Organocatalytic oxidations and reduction reaction.(4,5,6)

**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 member 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

**Optional Course**

**Inorganic Chemistry-V  
(Inorganic Spectroscopy)  
CYL-568**

**Credit 3-0-0**

- 1. Nuclear Quadruple Resonance Spectroscopy (5 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  $^{57}\text{Fe}$ ,  $^{119}\text{Sn}$ , complications like unusual intensities, non zero asymmetry parameter recoil fraction, magnetic ordering and relaxation. (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, methyl radical,  $\text{CH}_2\text{OH}$  cyclopentadienyl cycloheptatrienyl radical, pyrazine anion, pyrazine anion with  $^{23}\text{Na}$  and  $^{30}\text{K}$  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, hydrides, coupling to metals, Main group hydrides, transition metal hydrides, coupling to phosphine ligands, more than one hydride, coupling to metal, effect of trans ligand, dihydrogen complexes, Isotopes other than  $^1\text{H}$  e.g.  $^{31}\text{P}$ ,  $^{13}\text{C}$ ,  $^{14}\text{N}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ ,  $^{27}\text{Al}$ ,  $^{29}\text{Si}$ , transition metals. (books 1, 2 & 3)

**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. Craddock, Structural Methods in Inorganic Chemistry, Blackwell Scientific, Oxford, 1987.

**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]

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