

**COOCH BEHAR PANCHANAN BARMA UNIVERSITY**  
Syllabus for Post Graduate Course in Chemistry ( For the session 2020 –2021 )

**SYLLABUS for M.Sc in CHEMISTRY**

**(Course Duration : Four Semester – Two Year)**

**Total Credit : 80**

**Credit per Semester : 20**

**Total Marks = 1600**

**Theory = 700:**

**Practical = 300**

**Cont. Evaluation = 320**

**Viva/Seminar/Project = 200**

**Attendance = 80**

## Course Structure

Sem	Paper Code	Paper Name	Theo	CE	Attend	Total	Credit	Pract	Viva/ Seminar/ Project	Credit	Total Marks	Total Credit
Semester - 1	Core-1	Organic Chemistry-1	50	20	5	75	3	25		2	100	5
	Core-2	Inorganic Chemistry-1	50	20	5	75	3	25		2	100	5
	Core-3	Physical Chemistry-1	50	20	5	75	3	25		2	100	5
	Core-4	Spectroscopy	50	20	5	75	4	25		1	100	5
Semester - 2	Core-5	Organic Chemistry-2	50	20	5	75	3	25		2	100	5
	Core-6	Inorganic Chemistry-2	50	20	5	75	3	25		2	100	5
	Core-7	Physical Chemistry-2	50	20	5	75	3	25		2	100	5
	Core-8	Advanced Spectroscopy	50	20	5	75	4	25		1	100	5
Semester - 3	Core-9	Org/Inorg	50	20	5	75			25		100	5
	DCE-1	Organic/Inorganic/ Physical Special	50	20	5	75			25		100	5
	DCE-2	Organic /Inorganic /Physical (practical)		20	5			50	25	5	100	5
	GE-1	one from pool of three	50	20	5	75	3		25	2	100	5
Semester - 4	Core-10	Phy- Analytical & Industrial	50	20	5	75			25		100	5
	DCE-3	Organic /Inorganic /Physical Special	50	20	5	75			25		100	5
	DCE-4	Organic /Inorganic /Physical Special (practical)		20	5			50	25		100	5
	GE-2	one from pool of three	50	20	4	75	3		25	2	100	5
											1600	80

## Course Content

### Semester – I

### Organic Chemistry

**Paper Name : Organic Chemistry – I, Credit-5, FM-100**

**Paper Code : Core-1T**

**Theory (T) : Credit – 3, Full Marks – 75 (ESE -50 + CE- 20 + Attendance-5)**

#### **A. Structure Activity Relationship (18 Lectures)**

MO treatment of acyclic and cyclic conjugated systems; Hückel's rule and concept of aromaticity, annulenes, heteroannulenes, fullerenes ( $C_{60}$ ), alternate and non-alternate hydrocarbons, anti-aromaticity, pseudo-aromaticity, homo-aromaticity; graphical methods – Frost diagram, Hückel treatment - applications to ethylene, allyl cyclopropenyl, butadiene, cyclobutadiene.

#### **B. Stereochemistry (18 lectures)**

Acyclic systems up to 4 chiral centers : Compounds with asymmetric carbons in branched chains, symmetry; point groups, correlation of axial dissymmetry and centrodissymmetry, Nomenclature of compounds involving axial and planar chirality, Winstein-Holness equation, Curtin Hammett principle; Conformational analysis of cyclohexene, decalins and their derivatives; Effects of conformation on reactivity in acyclic compounds and cyclohexanes. Elements of Symmetry and Chirality, Optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis.

Criteria for Chirality. Desymmetrization. Axial, planar and helical chirality: Configurational nomenclature: Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, atropisomerism. Planar chiral ansa compounds and trans- cyclooctene. Helically chiral compounds

Relative and absolute configuration: Determination of absolute configuration by chemical correlation methods. Racemisation, racemates and resolution techniques: Resolutions by direct crystallization, diastereoisomer salt formation chiral chromatography and asymmetric transformation. Determination of configuration in E,Z-isomers: Spectral and Chemical methods of configuration determination of E,Z isomers. Determination of configuration in aldoximes and ketoximes

#### **C. Substitution & Elimination Reaction: (10 lectures)**

**substitution** (aliphatic electrophilic & nucleophilic) & **Elimination reactions** of aliphatic and aromatic compounds

#### **D. Pericyclic Reaction (14 lectures)**

Classification and stereochemical modes. Thermal and photopericyclic reactions, Selection rules and stereochemistry of electrocyclic reactions, cycloadditions, sigmatropic rearrangements, carbene addition, cheletropic reactions. Rationalization based on Frontier M.O. approach, correlation diagrams, Dewar-Zimmermann approach, Mobius and Hückel systems, Sommelet-Hauser, Cope, aza

Cope and Claisen rearrangements, Ene Reaction, Wittig rearrangement, suitable examples of [(2π + 2π), (4π + 2π), (4π + 4π), (2π + 2π + 2π)] and metal catalysed cycloaddition reactions.

**Paper Name : Organic Chemistry– I**

**Paper Code : Core-1P**

**Practical (P) :**

**Credit – 2,**

**Full Marks – 25**

**Practical**

**(30 practical classes)**

**Isolation of Natural products (Any three)**

1. Extraction of curcumin from turmeric.
2. Extraction of caffeine from tea/coffee.
3. Extraction of cinnamaldehyde from cinnamon
4. Extraction of Eugenol from clove
5. Extraction of Lycopene from tomatoes

**One stage preparations and Recrystallisation (any Ten)**

1. Benzilic acid rearrangement: Benzilic acid from benzil
2. Sandmeyer reaction: p-Nitroiodobenzene from p-nitroaniline
3. Heterocyclic compound: 7-Hydroxy-4-methylcoumarin from resorcinol
4. Acetylation: Mannitol hexaacetate from mannitol  
Acetanilide from Aniline.  
Glucose pentacetate from glucose
5. Claisen-Schmidt reaction Dibenzalacetone from benzaldehyde
6. Oxidation: Fluorenone from fluorine  
Benzoic acid from Benzaldehyde
7. Acetylation: Acetylferrocene from ferrocene
8. Hydrolysis: Benzoic acid from Benzamide.
9. Bromination: p-Bromoacetanilide from Acetanilide.
10. Nitration: m-dinitrobenzene from Nitrobenzene.  
p-nitroacetanilide from acetanilide
11. Benzoylation: Benzanilide from Aniline.

**Suggested Books**

- Adam Jacobs, Understanding organic reaction mechanism. Cambridge University press (1997)
- F.A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers (2000)
- E.L.Eliel, Stereochemistry of carbon compounds. John Wiley (1997)
- Modern Organic Synthesis-an introduction by George S. Zweifel and Michael H. Nantz, W. H. Freeman & company, New York
- Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
- Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sundberg, Fourth edition, Kluwer academic publishers, New York.
- Photochemistry and Pericyclic Reactions by Jagdamba Singh
- Organic Reactions and Orbital Symmetry by Gilchrist and Storr

**Paper Name : Inorganic Chemistry – I,**

**Paper Code : Core - 2T**

**Credit - 5,**

**FM-100**

**Theory (T) : Credit – 3, Full Marks – 75 (ESE -50 + CE- 20 + Attendance-5)**

- A. Coordination Chemistry: (18 lectures)**  
Adjusted CFT, Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stabilization of complexes (Irving Williams order). Site preference in mixed metal oxides (Spinel and inverse spinel structures). Tetrahedral distortion and Jahn Teller effect, Static and Dynamic Jahn-Teller effect. Microstates, Russell-Sander's terms, energy ordering of terms and Racah parameters, interelectronic repulsion parameters in complex ion terms-vs-free ion terms, hole formalism, determination of ground and excited state terms of  $d^n$  ions, spin-orbit coupling, effect of crystal field on Russell-Sander's terms, concept of correlation diagram.
- B. Structure & Bonding of Inorganic molecule (10 lectures)**  
Bonding in homonuclear and heteronuclear diatomic molecules of 2nd period. Bonding in triatomic ( $H_3^+$ ,  $BeH_2$ ,  $H_2O$ ), tetra-atomic ( $BH_3$ ,  $NH_3$ ) and  $CH_4$ . MO diagrams, Walsh diagrams. Models of structure prediction
- C. Reaction Mechanism-I: (18 lectures)**  
Inert and labile complexes, consideration of octahedral substitution reactions in the light of VBT and CFT. Mechanism of substitution reactions, Classification of reactions of complex compounds, energy profile diagram of ligand substitution reactions- associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution
- D. Clusters-I (12 lectures)**  
Higher boranes, carboranes, metalloboranes and metallocarboranes.

**Paper Name : Inorganic Chemistry–I**

**Paper Code : Core-2P**

**Practical (P) : Credit – 2, Full Marks – 25**

Inorganic qualitative analysis: Less common metals – Be, Mo, W, Ti, Zr, Th, V, U, Ce and all the radicals included in the B. Sc (Honours) Chemistry syllabus. (30 Classes)

**Suggested Books**

- Ligand field theory and its application by B. N. Figgis
- Inorganic chemistry, principal of structure and reactivity by J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi
- Inorganic Chemistry, 4th edition by C. E. Housecroft, A. G. Sharpe
- Inorganic Chemistry by Shriver and Atkins
- Inorganic Chemistry, Vol.- 5 by A. K. Das, M. Das
- Elements of magnetochemistry by R. L. Dutta, A. Shyamal
- Chemistry of elements by N. N. Greenwood and A. Earnshaw
- Inorganic Chemistry: Principles, D. Banerjee
- Hand book of Inorganic analysis, G. N. Mukherjee
- Vogel's Quantitative Inorganic analysis, G. Svehla & B. Shivasankar

**Paper Name : Physical Chemistry (T + P) – I, Credit-5, FM-100**

**Paper Code : Core-3T**

**Theory (T) : Credit – 3, Full Marks – 75 (ESE -50 + CE- 20 + Attendance-5)**

**A. Quantum Chemistry – I**

**(25 Lectures)**

Schrödinger equation, Basic postulates and theorems, Physical interpretation of wave function, stationary states, operator formation, atomic unit system, Heisenberg's equation of motion, Particle in a box problem, Finite barrier problem and tunneling, Linear harmonic oscillator, Ladder operators, Angular momentum problem, Rigid rotor. Hydrogen atom problem and its implications

**B. Classical Thermodynamics**

**(10 Lectures)**

Brief review of 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> laws of thermodynamics, Nernst heat theorem and the third law of thermodynamics, calculation of entropy changes in chemical reactions. Mathematical and thermodynamic probability, Entropy and probability, the free energy of a mixture, Partial molal quantities, Analytical form of the chemical potential in ideal solutions, Chemical potential of a solute in a binary solution, Application of Gibbs Duhem equation, Nonideal solutions, concept of activity: experimental determination of activity coefficients of non electrolytes, Application of thermodynamics to micelles and microemulsion

**C. Chemical Kinetics – I**

**(16 Lectures)**

Potential energy surface: reaction coordinates and reaction paths, Transition state theory and thermodynamics, Reactions in solutions: enzyme catalysis and enzyme inhibition reactions, ionic reactions, oscillating reaction.

Fast reactions: Flow and stop-flow technique, Flash photolysis, Relaxation and Nuclear magnetic resonance techniques

**D. Macromolecules**

**(13 Lectures)**

Polymer definition, various types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics and mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination by various methods (osmometry, viscometry, diffusion and light scattering), sedimentation, chain configuration of macromolecules, and calculation of average dimensions of various chain structures, visco-elasticity

**Paper Name : Physical Chemistry (T + P)– I**

**Paper Code : Core-3P**

**Credit – 2,**

**Full Marks – 25**

**Practical**

**(32 classes)**

1. Studies on the kinetics of iodination of acetone.
2. Determination of solubility product of  $PbI_2$  by titrametric method.
3. Determination of coordination number of  $Cu^{++}$  (partition method).
4. Ion exchange capacity of resin.
5. Verification of Beer's law and studies on the kinetics of alkaline hydrolysis of crystal violet.
6. Conductometric titration of a mixture of acids.
7. Estimation of acid potentiometrically.
8. Estimation of acid pH metrically.

**Suggested Books**

- Quantum Chemistry by A B Sannigrahi
- Chemical Kinetics (3<sup>rd</sup> edition) Pearson Publisher by K. J. Laidler

- Polymer Science (3<sup>rd</sup> Edition) by V.R. Gowariker, N.V. Viswanathan, Jayadev Sreedhar
- A Textbook of Physical Chemistry, Vol 5, by K. L. Kapoor, McGraw Hill Publisher
- Introductory polymer chemistry, by G. S. Misra
- Text Book of Polymer Science, F.W. Billmeyer
- Chemical Thermodynamics (Classical, Statistical & Irreversible) by Hrishikesh Chatterjee
- Thermodynamics For Chemists by Samuel Glasstone
- Practical Physical Chemistry by Renu Gupta (New Age International Publisher)
- An Advanced Course in Practical Chemistry by A.K. Nad, B. Mahapatra, A. Ghoshal

**Paper Name : Spectroscopy**

**Credit-5, FM-100**

**Paper Code : Core-4T Theory (T) :**

**Full Marks – 75 (ESE -50 + CE- 20 + Attendance-5) Credit =4**

- A. Introduction to basic principles, Widths and Intensities of spectral transitions, Fourier transform, computer averaging techniques, LASERS. **(10 lectures)**
- B. **Microwave Spectroscopy:** **(15 lectures)**  
 Classifications of molecules based on moments of inertia, Rotational spectra, Rigid and non rigid rotor model, Selection rules, Spectral intensity, degeneracy and relative population of energy levels, Isotopic substitution. Symmetric top molecules
- C. **Infra-red Spectroscopy:** **(12 lectures)**  
 Vibrational and rotation-vibrational spectra, Simple harmonic oscillator model, Selection rules, Fundamentals and overtones, Hot bands, Q, P, and R branches, Chemical analysis by IR techniques
- D. **Raman Spectroscopy** **(14 lectures)**  
 Rayleigh and Raman scattering, Classical and Quantum theory of Raman effect, Stokes and anti-Stokes lines, rotational and vibrational Raman spectra, Mutual exclusion rule, Applications of Raman spectroscopy.
- E. **<sup>1</sup>H NMR.** **(24 lectures)**  
 Principle, instrumentation and different techniques (CW & FT) of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant (J), spin decoupling, spin tickling, classification of ABX, AMX, ABC, A<sub>2</sub>B<sub>2</sub> in proton NMR.

**Paper Name : Spectroscopy**

**Paper Code : Core-4P**

**Credit – 1,**

**Full Marks – 25**

IR Spectra of prepared organic and inorganic compounds/IR band assignment. **(15 lectures)**  
 [Curcumin, caffeine of tea/coffee, cinnamaldehyde, Eugenol, Lycopene. Cobalt acetylacetonate, cis and trans [Co(en)<sub>2</sub>Cl<sub>2</sub>], Co(salen), Cu(acac)<sub>2</sub>.H<sub>2</sub>O]

**Suggested Books**

- Organic Spectroscopy: Dyer & Silverstein
- Fundamentals of Molecular Spectroscopy : C. N. Banwell
- Fundamentals of photochemistry : K. K. Rohatgi-Mukherjee
- Introduction to Molecular spectroscopy: G M Barrow

## Semester – II

**Paper Name : Organic Chemistry – I, Credit-5, FM-100**

**Paper Code : Core-5T**

**Theory (T) :**

**Credit – 3, Full Marks – 75 (ESE -50 + CE- 20 + Attendance-5)**

- A. Photochemistry** (15 Theory class)  
Basic principles, Jablonski diagram, photochemistry of olefinic compounds, Cis-trans isomerisation, stereomutation Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di- $\pi$ -methane rearrangement, photochemistry of arenes, Photoreaction in solid state. Method of generation and detection (ESR) of radicals, radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, cyclisation of radicals, allylic halogenation, autooxidation
- B. Nucleophilic and Electrophilic Aromatic substitution:** (15 Theory class)  
Aromatic Nucleophilic substitution:  $SN_1(Ar)$ ,  $SN_2(Ar)$ , and benzyne mechanisms; evidence for the structure of benzyne. Von Richter rearrangement. Definition and types of ambident nucleophiles. The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction
- C. Reagents in organic synthesis** (15 Theory class)  
Use of following reagents in organic synthesis and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, LDA, DCC, Merrifield resin, Peterson's synthesis, Lawesson's reagent, Wilkinson's catalyst, Baker yeast., hypervalent organoiodines (introduction) and reagents of non-transition metals – Zn, Cd, Sm and In
- D. Selective Name Reactions:** (15 Theory class)  
Barton, Baylis Hillman reaction, Benzoin condensation, Chichibabin Reaction, Darzens reaction, Dieckman condensations, Grignard reactions. Henry reaction, Knoevenagel reaction, Mannich, McMurry, Perkin, Peterson olefination, Reformatsky and Reimer-Tiemann, Robinson Annulation. Stobbe, Stork enamine reaction and selective mono and di alkylation via enamines. Wittig and its modifications and other reactions, Oppenauer oxidation, Mitsunobu Reaction

**Paper Name : Organic Chemistry–4**

**Paper Code : Core-5P**

**Practical (P) : Credit – 2, Full Marks – 25**

**Practical (P) :**

**(30 practical class)**

### **Isolation / Estimation of natural products**

1. Extraction of clove oil from cloves.
2. Estimation of glucose by Folin Wu method.
3. Estimation of citral using hydroxylamine hydrochloride.
4. Estimation of saponification value of oil.



**Two stage preparations (any Ten)**

1. Benzaldehyde → Benzalacetophenone → Epoxide
2. 4-Nitro toluene → 4-Nitro benzoic acid → 4-Amino benzoic acid
3. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-Methyl-7-acetoxy coumarin
4. Hydroquinone → Hydroquinone diacetate → 1,2,4-Triacetoxy benzene
5. Acetanilide → p-Acetamidobenzene sulphonyl chloride → p-acetamidobenzenesulphonamide
6. p-Amino phenol → p-Acetyl amino phenol → p-Ethoxy acetanilide
7. p-Cresol → p-Cresyl benzoate → 2-Hydroxy-5-methyl benzophenone
8. Phthalimide → N-Benzylphthalimide → Benzylamine
9. Aniline → Acetanilide → p-nitroacetanilide
10. Acetanilide → p-nitroacetanilide → p-nitroaniline
11. benzyl alcohol → benzaldehyde → benzoic acid
12. Phthalic acid → Phthalimide → Anthranilic acid
13. o-Nitroaniline → o-Phenylene diamine → Benzimidazole
14. Aniline → Acetanilide → p-bromoacetanilide

**Suggested Books:**

- Photochemistry and Pericyclic Reactions by Jagdamba Singh
- Organic Reactions and Orbital Symmetry by Gilchrist and Storr
- Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
- Modern Organic Synthesis-an introduction by George S. Zweifel and Michael H. Nantz, W. H. Freeman & company, New York

**Paper Name : Inorganic Chemistry – II, Credit-5, FM-100**

**Paper Code : Core-6T**

**Theory (T) : Credit – 3, Full Marks – 75 (ESE -50 + CE- 20 + Attendance-5)**

**A. Metal-ligand equilibrium in Solution: (16 lectures)**

Stability of mononuclear, polynuclear and mixed ligand complexes in solution. Stepwise and overall formation constants and their relations. Trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of the metal ions and ligands. Statistical and non-statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed ligand complexes with reference to chelate effect and thermodynamic considerations. Macrocyclic and template effect. Spectrophotometric and pH metric determination of binary formation constants

**B. Spectra of Complex: (18 lectures)**

Orgel diagrams (qualitative approach), Tanabe-Sugano diagrams, selection rules for spectral transitions, relaxation of selection rule and band intensity, band width and shape, d-d spectra of  $d^n$  ions and crystal field parameters, measurement of  $10 Dq$  and  $B$ , nephelauxetic series, effect of Jahn-Teller distortion on spectra. Experimental evidence of metal-ligand overlap. MOT to rationalize  $\sigma$  and  $\pi$  interactions in octahedral, square planar and tetrahedral metal complexes. Symmetry designations of LGOs and MOs. Simplified MO diagrams

- C. Reaction Mechanism of inorganic complex: (20 lectures)**  
 Some important rate laws of ligand substitution reaction, activation parameters ( $\Delta S^\ddagger$ ,  $\Delta H^\ddagger$ ,  $\Delta V^\ddagger$ ), mechanism of isomerization reaction, linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms, substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc. conjugate base formation, anation reaction and base hydrolysis, reactions without metal-ligand cleavage. Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution process, nucleophilicity parameter.
- D. Clusters-II (8 lectures)**  
 Metal carbonyls and halide clusters, compounds with metal-metal multiple bonds, isopoly and heteropoly acids and their salts.

**Paper Name : Inorganic Chemistry–II**

**Paper Code : Core-6P**

**Practical (P) : Credit – 2, Full Marks – 20**

**Inorganic quantitative analysis: (15 lectures)**  
 Separation and estimation of two metal ions from minerals, alloys or solutions.

**Suggested Books**

- Ligand field theory and its application by B. N. Figgis
- Inorganic chemistry, principal of structure and reactivity by J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi
- Inorganic Chemistry, 4th edition by C. E. Housecroft, A. G. Sharpe
- Inorganic Chemistry by Shriver and Atkins
- Inorganic Chemistry, Vol.- 5 by A. K. Das, M. Das
- Inorganic Chemistry, Vol.- 6 by A. K. Das, M. Das
- Elements of magnetochemistry by R. L. Dutta, A. Shyamal
- Inorganic Chemistry: Principles , D. Banerjee
- Hand book of Inorganic analysis, G. N. Mukherjee
- Vogel's Text Book of Quantitative Inorganic analysis, J. Bassett, R.C Denny, G. H Jefery & J. Mendham

**Paper Name : Physical Chemistry (T + P)– II Credit = 5, F.M =100**

**Paper Code : Core-7T**

**Theory (T) : Credit – 3, Full Marks – 75 (ESE- 50 + CE- 20 + Attendance- 5)**

- A. Quantum Chemistry – II (28 lectures)**  
 The variational method, Eckart's theorem, Linear variational method, Perturbation theory (time independent), Application of variational method and nondegenerate perturbation theory to the helium atom problem. Electron spin, Antisymmetry principle, Spectroscopic term symbols, Spin-orbit coupling, Degenerate perturbation theory and its application to Zeeman and anomalous Zeeman effect, Stark effect.

**B. Computers for Chemists: (10 lectures)**

Fundamentals of Computers, Elements of the computer language (FORTRON, BASIC, C), Constants and variables, Operations and symbols, Expressions, Arithmetic assignment statement, Input and Output format statement, Termination statements, Branching statements. Branching statements such as IF or GO TO statements of LOGICAL variables, Double precision variables. Subscripted variables and DIMENSION DO statement FUNCTION and SUBROUTINE COMMON and DO Statement FUNCTION and SUBROUTINE COMMON and DATA statements (above language features refer to FORTRON; may be changed appropriately for C / BASIC)

Development of small computer codes involving simple formulae in chemistry, such as equations for kinetics, radioactive decay etc, Evaluation of lattice energy and ionic radii from experimental data, Linear simultaneous equations to solve secular equations within the Hijckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge than base

**C. Electrochemistry (27 lectures)**

Ion-association, Formation of ion-pairs, triplets etc; Ion-solvent interactions, The Born model, structural treatment of ion-solvent interactions, ion-quadruple theory of solvation, The solvation number, Debye-Hückel theory, Debye-Hückel-Onsagar theory, Electrophoretic and relaxation effects, Wein effects, Debye – Fulckenhegen effect.

**Paper Name : Physical Chemistry (T + P)– II**

**Paper Code : Core-7P, Credit =2**

**Practical : (15 lectures)**

1. Studies on alkalis hydrolysis of ethyl acetate conductometrically.
2. Determination of  $pK_1$  and  $pK_2$  of phosphoric acid potentiometrically.
3. Determination of  $pK_1$  and  $pK_2$  of phosphoric acid pH metrically.
4. Verification of Debye Hückel Onsager-equation.
5. Studies on the kinetics of reaction between  $K_2S_2O_8$  and KI spectrophoto-metrically.
6. Studies on the kinetics of reaction between  $KBr_3$  and  $KBr$  titrimetrically.
7. Potentiometric estimation of Fe (II) using  $K_2Cr_2O_7$ .
8. Ternary phase diagram of  $H_2O/C_6H_6/CH_2COOH$ .

**Suggested books**

- Quantum Chemistry by A B Sannigrahi
- Modern Electrochemistry-Vol-1 by John OM Bockris, Amulya K. N. Reddy
- Practical Physical Chemistry by Renu Gupta (New Age International Pubisher)
- An Advanced Course in Practical Chemistry by A.K. Nad, B. Mahapatra, A. Ghoshal

**Paper Name : Advanced Spectroscopy,**

**Credit = 5, F.M. = 100**

**Paper Code : Core-8T**

**Theory (T) : Credit – 4, Full Marks – 75 (ESE- 50 + CE- 20 + Attendance- 5)**

- A. Molecular Symmetry and Group theory (20 lectures)**  
Symmetry elements and symmetry operations, Group theory: definitions and theories, multiple symmetry operations, multiplication table, molecular point groups, Simple ideas of representation and character table, direct product.
- B. <sup>13</sup>C NMR spectroscopy; CD, ORD; ESR, Mössbauer & EXAFS (25 lectures)**
- C. NMR Spectroscopy of inorganic compounds (15 lectures)**  
1H NMR spectra of paramagnetic coordination compounds, dipolar and contact shifts, magnetic susceptibility and resonance shifts. <sup>11</sup>B, <sup>19</sup>F, <sup>27</sup>Al, <sup>31</sup>P, <sup>51</sup>V – NMR spectra. Pascal triangle, Contact shifts. Factors contributing the magnitude of chemical shift. NMR shift reagent and MRI reagent. Applications of NMR spectroscopy in inorganic systems.
- D. Fluorescence spectroscopy (15 lectures)**  
Principles of fluorescence spectra, Jabonlaski diagram, mirror image rule, intersystem crossing, selection of exciting wavelength, quantum yield, effect of temperature, solvent polarity and viscosity, quenching of fluorescence, inner-filter effect, fluorescence of biomolecules,

**Paper Name : Advanced Spectroscopy (T + P)**

**Paper Code : Core-8P, Credit = 1**

- A. Assignment of NMR peaks of selected organic and inorganic compounds (selected by the concerned teachers).
- B. collection of UV-visible spectra of the following compounds:  
[Curcumin, caffeine of tea/coffee, cinnamaldehyde, Eugenol and related organic compounds. synthesized nano particles, Cobalt acetylacetonate, cis and trans [Co(en)<sub>2</sub>Cl<sub>2</sub>], cis and trans Cu(glycinato)<sub>2</sub> CuSO<sub>4</sub>, Cu(acac)<sub>2</sub>.H<sub>2</sub>O and related inorganic compounds.]

**Suggested Books**

- Application of absorption spectroscopy of Organic Spectroscopy: J. R. Dyer
- Organic Spectroscopy: W. Kemp
- Fundamentals of Molecular Spectroscopy : C. N. Banwell
- Fundamentals of photochemistry : K. K. Rohatgi-Mukherjee
- Introduction to Molecular spectroscopy: G M Barrow
- Fundamental concepts of inorganic chemistry, vol - 7, A. D. De
- Physical methods in inorganic chemistry: R. S. Drago