

DEPARTMENT OF CHEMISTRY  
UNIVERSITY OF NORTH BENGAL



Enlightenment to perfection

**Distribution of Credits under CBCS in Two-years (4 Semesters) P.G. Course in Chemistry**

**New Syllabus for M. Sc (Regular) in Chemistry**

(Course Duration = Four-Semester Two-year)

**Total Credits = 64**

**Theory = 38 Credits**

**Practical = 10 Credits**

**Cont. Evaluation = 16 Credits**

Semester	Theory (T)			Practical (P)			Continuing Evaluation		Total		
	Course ID	Marks	Credit	Course ID	Marks	Credit	Marks	Credit	Marks	Credit	
I	Organic Chemistry (ORG)						CT/1 (Equal weightage)		100	4	
	ORG-T/01	50	3	ORG-P/02	50	1					
	Inorganic Chemistry (ING)										
	ING-T/01	50	3	ING-P/02	50	1					
	Physical Chemistry (PHY)										
	PHY-T/01	50	3	PHY-P/02	50	1					
<b>Marks / Credits</b>		<b>150</b>	<b>9</b>		<b>150</b>	<b>3</b>	<b>100</b>	<b>4</b>	<b>400</b>	<b>16</b>	
II	Organic Chemistry (ORG)						CT/2=100 (Equal weightage)		100	4	
	ORG-T/03	50	3	ORG-P/04	50	1					
	Inorganic Chemistry (ING)										
	ING-T/03	50	3	ING-P/04	50	1					
	Physical Chemistry (PHY)										
	PHY-T/03	50	3	PHY-P/04	50	1					
<b>Marks / Credits</b>		<b>150</b>	<b>9</b>		<b>150</b>	<b>3</b>	<b>100</b>	<b>4</b>	<b>400</b>	<b>16</b>	
III	IOP - T/05	100	5				CT/3& Seminar/Project		50 + 50	2 + 2	
	Organic Chemistry (ORG)										
	ORG-T/06	100	5	ORG-P/07	100	2					
	Inorganic Chemistry (ING)										
	ING-T/06	100	5	ING-P/07	100	2					
	Physical Chemistry (PHY)										
	PHY-T/06	100	5	PHY-P/07	100	2					
<b>Marks</b>		<b>200</b>	<b>10</b>		<b>100</b>	<b>2</b>	<b>100</b>	<b>4</b>	<b>400</b>	<b>16</b>	

<b>IV</b>	<b>Organic Chemistry (ORG)</b>						<b>CT &amp; Project / Dissertation</b>			
	ORG-T/08 ORG-T/09	100 100	5 5	ORG-P/10	100	2	50 +50	2+2		
	<b>Inorganic Chemistry (ING)</b>									
	ING-T/08 ING-T/09	100 100	5 5	ING-P/10	100	2				
	<b>Physical Chemistry (PHY)</b>									
	PHY-T/08 PHY-T/09	100 100	5 5	PHY-P/10	100	2				
	<b>Marks</b>	<b>200</b>	<b>10</b>		<b>100</b>	<b>2</b>	<b>100</b>	<b>4</b>		
<b>Total Marks</b>	<b>700</b>	<b>38</b>		<b>500</b>	<b>10</b>	<b>400</b>	<b>16</b>	<b>1600</b>	<b>64</b>	

\*CT = Class Test

**Course Content**  
**Inorganic Chemistry**

**Semester-I**

<u>Course ID- ING-T/01</u>	<b>Number of Classes</b>
<p><b>A: Organometallic compounds of main group elements – I</b></p> <p>Synthesis, properties and structures of organometallic compounds of group-I to group-III elements of the periodic table.</p>	<b>15</b>
<p><b>B: Clusters-I</b></p> <p>Higher boranes, carboranes, metalloboranes and metallocarboranes.</p>	<b>20</b>
<p><b>C: Reaction mechanism of transition metal complexes-I</b></p> <p>Classification of reactions of complex compounds, inert and labile complexes, consideration of octahedral substitution reactions in the light of VBT and CFT, 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, some important rate laws, activation parameters (<math>\Delta S^\ddagger</math>, <math>\Delta H^\ddagger</math>, <math>\Delta V^\ddagger</math>), 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.</p>	<b>20</b>
<p><b>D: Magnetic properties and spectra-I</b></p> <p>Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, Russell-sander's terms, determination of magnetic susceptibility, magnetic properties of first transition series metal ions and lanthanides.</p>	<b>20</b>
<u>Course ID- ING-P/02</u>	<b>75</b>
<p>Inorganic qualitative analysis:</p> <p>Less common metals – Be, Mo, W, Ti, Zr, Th, V, U, Ce and all the radicals included in the B. Sc (Honours) Chemistry syllabus.</p>	

## Semester-II

<u>Course ID</u> - <b>ING-T/03</b>	<b>Number of Classes</b>
<p><b>A: Organometallic compounds of main group elements-II</b></p> <p>Synthesis, properties and structures of organometallic compounds of group-IV &amp; V elements of the periodic table.</p>	<b>20</b>
<p><b>B: Reaction mechanism of transition metal complexes-II</b></p> <p>Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution process, nucleophilicity parameter, etc. Redox reactions- complementary and non-complementary reactions, mechanisms of outer sphere and inner sphere electron transfer reactions, theory of outer sphere processes, the Marcus cross relation.</p>	<b>20</b>
<p><b>C: Clusters-II</b></p> <p>Metal carbonyls and halide clusters, compounds with metal-metal multiple bonds, isopoly and heteropoly acids and their salts.</p>	<b>20</b>
<p><b>D: Magnetic properties and spectra-II</b></p> <p>CFT and its limitations, Orgel diagrams and spectra, calculations of <math>Dq</math>, <math>B</math> and <math>\beta</math> - parameters, charge transfer spectra, anomalous magnetic moment, magnetic exchange coupling and spin crossover.</p>	<b>20</b>
<p><u>Course ID</u> - <b>ING-P/04</b></p> <p>Inorganic quantitative analysis: Separation and estimation of two metal ions from minerals, alloys or solutions.</p>	<b>80</b>

**Semester-III****Number of Classes****Common Paper**Course ID - IOP - T/05**A: Analytical Chemistry: 5**

- Recapitulation of the elementary concepts of Analytical Chemistry.
- Selected analytical techniques:
  - ∅ Solvent extraction.
  - ∅ High performance liquid chromatography (Brief ideas).

**B: NMR Spectroscopy 7**

Introduction to the techniques and Application of NMR:  $^1\text{H}$  and  $^{13}\text{C}$  NMR - principles, instrumentation; principles of decoupling, gated and inverse gated decoupling, NOE, relaxation process, selective polarization transfer, INEPT, basic two-dimensional sequence, homonuclear and heteronuclear shift correlation.

**C: Organometallic Reagents 8**

Principle, preparations, properties and application of organometallic compounds of transition elements – Cu, Pd, Ni, Fe, Co, Rh, Ru, Cr and Ti in organic synthesis and in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerization), structure and mechanistic aspects, Davies rule, catalytic nucleophilic addition and substitution reaction, coupling reaction – Heck, Stille, Suzuki coupling, Sonogashia, Buchwald-Hartwig, Ziegler Natta reaction, Walker Process, Olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, functional organometallic compounds, pi-acid metal complexes, activation of small molecules by coordination.

**D: Reagents in organic synthesis 5**

Use of following reagents in organic synthesis and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, LDA, DCC, 1,3 - Dithane (reactivity umpolung). Merrifield resin, Peterson's synthesis, Laweson's reagent. Wilkinson's catalyst, Baker yeast., hypervalent organo iodines (introduction) and reagents of non transition metals – Zn, Cd, Sm and In.

**E: Advanced Quantum Chemistry 7**

Many electron treatment, Pure-spin states, Slates-Condon rules, Hartree-Fock theory, Hartree-Fock-Roothaan method.

	<b>Number of Classes</b>
<b>F: Group theoretical representation and spectroscopy</b>	<b>4</b>
Reducible and irreducible representations, classes and characters, Great Orthogonality and related theorems.	
<b>G: Polymer Chemistry</b>	<b>4</b>
Theory of polymers solutions, entropy and Flory-Huggins theory, Commercial polymer and bio-medical applications, Polyethylene, polyvinyl chloride, polyamides, polyester, phenolic resins epoxy resins and silicone polymers, Functional polymers-Fire retarding polymers and electrically conducting polymers.	
<u>Course ID - ING-T/06</u>	
<b>A: Organotransition Metal Chemistry-I</b>	<b>5</b>
<ul style="list-style-type: none"> <li>• Alkyls and aryls of transition metals.</li> <li>• Compounds of transition metal-carbon multiple bonds.</li> <li>• Transition metal-<math>\pi</math> -complexes.</li> </ul>	
<b>B: Chemical Bonding-I</b>	<b>10</b>
Crystal field theory- splitting of d- orbitals in electrostatic fields of different symmetry, $10Dq$ value, spectrochemical series, structural effects of CF splittings- ionic radii, Jahn Teller effects, thermodynamic effect of CF splitting- hydration, ligation and lattice energies, Irving-William series of formation constants, site preference in mixed metal oxides (Spinel and inverse spinel structures), defect of CFT, experimental evidence for metal-ligand overlap, MOT for bonding in complex compounds including $\sigma$ - and $\pi$ -bonding, comparison of VBT, CFT and MOT (Application of group theory as and when needed in the above cases).	
<b>C: Bio-inorganic Chemistry-I</b>	<b>5</b>
Metal ions in biological systems, essential and trace elements, Transport and storage of dioxygen: hemoglobin, myoglobin, hemerythrin and hemocyanine. Electron transfer in biology: Structure and functions of metalloproteins in electron transfer process: iron-sulfer proteins, cytochromes.	
<b>D: Photoinorganic Chemistry:</b>	<b>5</b>
Basics of photochemistry, properties of excited states, excited states of metal complexes, ligand field photochemistry, redox reactions by excited metal complexes, metal complex sensitizers, photo-splitting of water and solar energy conversion/storage.	

	<b>Number of Classes</b>
<b>E: Solid State Chemistry-I</b>	<b>5</b>
Electronic properties and Band theory in relation to selected inorganic compounds.	
<b>F: Spectrometric Techniques:</b>	<b>5</b>
Characterization of inorganic compounds by vibrational, rotational spectroscopy, ESR, Mössbauer & EXAFS.	
<b>G: Chemistry of:</b>	<b>5</b>
i) Actinides.	
ii) Boranes and their related compounds.	

Course ID - ING-P/07

### **Inorganic Practical**

**50**

1. Preparation of inorganic compounds/complexes and their physico-chemical characterization by different spectroscopic (IR, UV-Visible, NMR, etc) and magnetic susceptibility measurements. Depending on the availability of reagents and instruments compounds/complexes will be selected from the list given below:

Stannic iodide, sodium tetrathionate, transition metal acetylacetonates, *cis*- and *trans*-dichloro-bis(ethylenediamine) cobalt(III) chloride, tris(ethylenediamine) cobalt(III) chloride, chloro pentaamino cobalt(III) chloride, nitro pentaamino cobalt(III) chloride, nitrito pentaamino cobalt(III) chloride, *ortho*- and *para*- hydroxy mercury (II) chloride, *cis* and *trans* bis(glycinato) copper (II), polydentate ligands and their transition metal complexes specially of Ru, Rh, Re and Pt, some air and moisture-sensitive inorganic compounds.

**30**

2. Hydrothermal synthesis of metal-organic hybrid compounds and study on their physico-chemical properties. Experiments will be set depending upon the availability of instruments and reagents.

**Semester-IV****Number of Classes****Course ID - ING-T/08****A: Advanced Analytical Chemistry** **6**

Selected Analytical Techniques:

- Spectrophotometry.
- Thermal methods of analysis.
- Electro-analytical techniques.
- Radioactive methods of analysis.
- Fluorimetry, nephelometry, turbidometry and atomic absorption spectroscopy.

**B: Bio-inorganic Chemistry-II** **10**Photosynthesis: PS-I & PS-II, nitrogenase, metal ion storage and transport, metalloenzymes, Na<sup>+</sup>/K<sup>+</sup> pumps.**C: Molecular spectroscopy** **4**

- Hamiltonian in presence of electric and magnetic field, interaction with electromagnetic radiation, induced emission and absorptions, the Einstein transition probabilities.
- Electronic absorption spectroscopy- potential energy curves, Franck-Condon principle, oscillator strength, selection rules and intensity of electronic transitions, charge transfer spectra.

**D: Chemistry of the missing elements.** **4****E: Organotransition metal chemistry-II** **8**

- Transition metal compounds with bonds to hydrogen.
- Organometallic catalysts.
- Fluxional organometallic compounds.

**F: Characterization of inorganic compounds by NMR, ORD/CD & ESCA.** **8****Course ID - ING-T/09****A: Chemical bonding-II** **12**Charge transfer spectra, electron absorption spectra, d<sup>1</sup> and d<sup>9</sup> systems, multi-electron systems, Tanabe-Sugano diagrams for various d<sup>n</sup>- configurations, ACFT.



	<b>Number of Classes</b>
<b>B: Chemistry of Non-transitional Elements:</b>	<b>6</b>
Compounds with B-N bonds, P-N bonds and S-N bonds.	
<b>C: Solid state chemistry-II</b>	<b>9</b>
Crystal defects and non-stoichiometry of inorganic compounds, colour centre, photographic process, phosphors.	
<b>D: Crystal morphology:</b>	<b>9</b>
Important minerals and different types of silicates: structural and physical properties.	
<b>E: Chemistry of materials:</b>	<b>4</b>
<ul style="list-style-type: none"> <li>i) Inorganic supramolecular chemistry: Basic terms and concepts, nature and types of supramolecular forces, self-assembly of metal atoms/coordination, metal-organic frameworks (MOFs).</li> <li>ii) Nanomaterials: Fundamental physical and chemical principles, characterization, fabrication and applications.</li> </ul>	

Course ID - ING-P/10

**Inorganic Practical**

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|---|-----------|
| 1) Quantitative analysis.   | <b>50</b> |
| 2) Quantitative estimation of metal concentration at trace level by spectroscopic techniques (UV-Visible and atomic absorption spectroscopy). | <b>30</b> |

## Organic Chemistry

### Semester – I

#### Number of Classes

Course ID - ORG-T/01

**A: Structure Activity Relationship** **10**

MO treatment of acyclic and cyclic conjugated systems; Huckel's rule and concept of aromaticity, annulenes, heteroannulenes, fullerenes (C<sub>60</sub>), alternate and non-alternate hydrocarbons, anti-aromaticity, pseudoaromaticity, homo-aromaticity; graphical methods – Frost diagram, Huckel treatment - applications to ethylene, allyl cyclopropenyl, butadiene, cyclobutadiene.

**B: Stereochemistry – I** **10**

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.

**C: Substitution (aliphatic electrophilic & nucleophilic) & Elimination reactions** **10**

Phase transfer catalysis; ultrasound, ambient nucleophile, regioselectivity.

**D: Pericyclic Reaction** **15**

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 Huckel systems, Sommelet-Hauser, Cope, aza Cope and Claisen rearrangements, Ene Reaction, Wittig rearrangement, suitable examples of [(2 $\pi$  + 2 $\pi$ )], (4 $\pi$  + 2 $\pi$ ), (4 $\pi$  + 4 $\pi$ ), (2 $\pi$  + 2 $\pi$  + 2 $\pi$ ) and metal catalysed cycloaddition reactions

**E: Spectroscopy – I** **15**

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. Elementary principles of ESR, EPR and mass spectral techniques.

<b>F: Natural Products – I</b>	<b>Number of Classes</b>
	<b>15</b>

Isoprene rule, Structure elucidation (by chemical and spectroscopic methods), Synthesis, Biogenesis and Biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes, Structural types; general introduction to sesqui-, di- and tri-terpenoids.

<b><u>Course ID- ORG -P/02</u></b>	<b>75</b>
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Identification of single organic liquid with one or more functional groups : purification of organic sample by distillation / vacuum distillation / fractional vacuum distillation, determination of boiling point, solubility analysis and classification, functional group analysis, derivatization and complete identification, use of spectroscopic techniques (IR, UV, NMR).

### Semester – II

**Course ID - ORG -T/03**

<b>A: Photochemistry</b>	<b>12</b>
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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>B: Synthetic Strategy</b>	<b>12</b>
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Retrosynthetic analysis, disconnection approach, Typical examples to illustrate the disconnection approach, Functional group interconversion, Umpolung (1,3-dithiane), Convergent synthesis.

<b>C: Spectroscopy - II</b>	<b>15</b>
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Introduction to <sup>13</sup>C NMR spectroscopy; theoretical treatment of rotational, vibrational and electronic spectroscopy, principles of photoelectron spectroscopy. Application of electronic, vibrational, NMR, ESR, EPR and mass spectral techniques to simple structure and mechanistic problems.

<b>D: Stereochemistry – II</b>	<b>15</b>
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Correlation of axial dissymmetry and centrodissymmetry, nomenclature of compounds involving axial and planar chirality, dynamic stereochemistry.

	Number of Classes
<b>E: Reaction Kinetics &amp; Mechanism:</b>	<b>10</b>
(a) Labelling and Kinetic isotope effects, Hammett, Hanch and Taft equations, sigma-rho relationship , (b) Non classical carbonium ions. (c) Thermodynamic & kinetic requirement, kinetic & thermodynamic control.	

<b>F: Natural Products – II</b>	<b>16</b>
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Familiarity with methods of structure elucidation (chemical & spectroscopical method), biosynthesis, synthesis and biological activity of the alkaloids - nicotine, atropine, coniine and papaverine.

<u>Course ID - ORG -P/04</u>	<b>80</b>
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Organic preparation involving Aldol condensation, aromatic substitution reaction, Sandmeyer reaction, Friedel-Crafts reaction.

Quantitative analysis - Estimation of Phenol, Glucose & Sucrose. Determination of  $pK_a$  of benzoic acid.

### Semester III

#### Common Paper

#### Course ID - : IOP - T/05

<b>A: Analytical Chemistry:</b>	<b>5</b>
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- Recapitulation of the elementary concepts of Analytical Chemistry.
- Selected analytical techniques:
  - ∅ Solvent extraction.
  - ∅ High performance liquid chromatography (Brief ideas).

<b>B: NMR Spectroscopy</b>	<b>7</b>
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Introduction to the techniques and Application of NMR:  $^1\text{H}$  and  $^{13}\text{C}$  NMR - principles, instrumentation; principles of decoupling, gated and inverse gated decoupling, NOE, relaxation process, selective polarization transfer, INEPT, basic two-dimensional sequence, homonuclear and heteronuclear shift correlation.

<b>C: Organometallic Reagents</b>	<b>8</b>
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Principle, preparations, properties and application of organometallic compounds of transition elements – Cu, Pd, Ni, Fe, Co, Rh, Ru, Cr and Ti in organic synthesis and in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerization), structure and mechanistic aspects, Davies rule, catalytic nucleophilic addition and substitution reaction, coupling reaction – Heck, Stille, Suzuki coupling, Sonogashia, Buchwald-Hartwig, Ziegler Natta reaction, Walker

**Number of Classes**

Process, Olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, functional organometallic compounds, pi-acid metal complexes, activation of small molecules by coordination.

**D: Reagents in organic synthesis** **5**

Use of following reagents in organic synthesis and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, LDA, DCC, 1,3 - Dithane (reactivity umpolung). Merrifield resin, Peterson's synthesis, Laweson's reagent. Wilkinson's catalyst, Baker yeast., hypervalent organo iodines (introduction) and reagents of non transition metals – Zn, Cd, Sm and In.

**E: Advanced Quantum Chemistry** **7**

Many electron treatment, Pure-spin states, Slates-Condon rules, Hartree-Fock theory, Hartree-Fock-Roothaan method.

**F: Group theoretical representation and spectroscopy** **4**

Reducible and irreducible representations, classes and characters, Great Orthogonality and related theorems.

**G: Polymer Chemistry** **4**

Theory of polymers solutions, entropy and Flory-Huggins theory, Commercial polymer and bio-medical applications, Polyethylene, polyvinyl chloride, polyamides, polyester, phenolic resins epoxy resins and silicone polymers, Functional polymers-Fire retarding polymers and electrically conducting polymers.

Course ID - ORG -T / 06**A: Stereochemistry – III** **6**

Chiroptical properties of Organic Molecules: Origin, Theory. CD, ORD – VCD- principles and applications, haloketone rules, sector rules, helicity rules.

**B: Advanced Heterocyclic Chemistry – II** **6**

Indoles, pyrimidines, pyridazines, pyrazines, purines, pteridines compounds. Role of heterocyclic compounds in biological systems.

**C: Metallocenes, non benzenoid aromatics and polycyclic aromatic compounds,** **8**

Bonds weaker than covalent – addition compounds, crown ether, complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

	<b>Number of Classes</b>
<b>D: Natural Products – III</b>	<b>8</b>
Structure and Chemistry of quinoline alkaloids with special reference to cinchona group; isoquinoline alkaloids – morphine group.	

**E: Synthetic Methodology**

Organoboron – Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes, unsaturated hydrocarbon synthesis, allyl boranes, boron enolates.	<b>6</b>
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Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Wittig, Stobbe reaction, hydrolysis of esters and amides, ammonolysis of esters, addition to C - C & C - N multiple bonds.	<b>6</b>
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Course ID - ORG-P / 07

Organic multi-step preparations by the use of organic reagents and purification of the products by chromatographic techniques.	<b>40</b>
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Extraction of Natural products & their purification (Thin layer and Column Chromatography) and partial characterization by IR, UV and NMR.	<b>40</b>
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**Semester – IV**Course ID - ORG –T / 08

<b>A: Spectroscopy – III</b>	<b>10</b>
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Application of DEPT,  $^1\text{H}$ - $^1\text{H}$  COSY, HETCOR, TOCSY, NOESY in structure elucidation of organic compounds, drug screening, reaction monitoring etc. q - NMR & DOSY.

<b>B: Bio-Organic Chemistry</b>	<b>10</b>
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Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality, Biomimetic chemistry, crown ethers, Cyclodextrins, cyclodextrin-based models, calixarenes, ionophores, micelles, synthetic enzymes or synzymes.

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and Biological functions of coenzymes A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, EMN, FAD, lipoic, vitamin B<sub>12</sub>. Mechanisms of reactions catalyzed by the above cofactors.

<b>C: Spectroscopy - IV</b>	<b>8</b>
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Modern techniques of mass spectroscopy: FAB, MIKE LCMS / MS, ES / MS, MS-MS.

	<b>Number of Classes</b>
<b>D: Natural Products –IV</b>	<b>12</b>
Steroids: Occurrence, nomenclature, basic skeleton, and stereochemistry; Synthetic principles and chemical reactions.	
Plant Pigments: Synthesis and reactions of Coumarin and Chromones; occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteolin, Quercetin, Myrcetin Quercetin 3-glucoside, Vitexin, Diadzein, Butulin , Aureusin , Cyanidin-7-arabinoside, Cyanidin, Hirsutidin.	
Biosynthesis of flavonoids: Acetate pathway and shikimic and pathway.	

Course ID - ORG -T / 09**A: Green Chemistry** **10**

Green Chemistry – Overview, Set of Principles of Green Chemistry, Green synthetic methods, Catalytic methods, Organic synthesis in aqueous media, Ionic liquid, Supercritical fluids and microwave, Solvent free organic reactions, solid phase organic synthesis.

**B: Nucleoside & Nucleotide** **10**

Chemical synthesis of nucleosides and oligonucleotides; Biosynthesis of nucleotides and folic acids; Replication, transcription, protein biosynthesis, Covalent interactions of nucleic acids with small molecules, Structural features of DNA and RNA.

**C: Compounds of non metals** **10**

Chemistry of Organo sulphur, Organo phosphorus and organo silicon compounds.

**D: Natural Products – V** **10**

Structure, transformations, synthesis of simple and monoterpenoid derived indole alkaloids - reserpine, strychnine, ellipticine, lysergic acid, abiatic acid.

Course ID - ORG-P / 10

Separation and identification of the components of a binary mixture of organic solids: chromatographic separation, purification and identification of individual components (use of IR, UV, NMR), derivatization of individual component and analytical establishment of their identity. **50**

Multi-step organic preparations, Organoanalytical experiments / Project work. **30**

## Physical Chemistry

### Semester - I

#### Number of Classes

Course ID - PHY-T/01

**A: Quantum Chemistry I** **25**

Schrödinger equation, Basic postulates and theorems, Physical interpretation of wave function, stationary states, operator formalism, 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**

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** **10**

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** **20**

Polymer definition, various types of polymers, kinetics and mechanism of polymerization and oscillation reactions Molecular mass, number and mass average molecular mass, molecular mass determination by various methods (osmometry, viscometry, diffusion and light scattering)

**E: Introduction to spectroscopy:** **10**

Basic principles, Electronic, Vibrational and rotational spectra, Linear oscillator, rotator models, Selection rules, Rayleigh scattering and Raman spectroscopy, Application of UV, IR, Microwave, Raman spectroscopy to chemical analysis, Lasers.



Course ID - PHY-P/02:**Number of Classes**  
**75****Practical**

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.

**Semester- II**Course ID - PHY – T / 03**A: Quantum Chemistry II****24**

The variational method, Eckart's theorem, Linear variational method, Perturbation theory (time dependent), 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. Huckel M.O. theory for conjugated systems, bond order and charge density calculations, Introduction to the method of self consistent Field, Hartree method, Koopman's theorem.

**B: Molecular Symmetry and Group theory****10**

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.

**C: Computers for Chemists****26**

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

**Number of Classes**

structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge than base.

**D: Electrochemistry** **10**

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-Huckel theory, Debye-Huckel-Onsagar theory, Electrophoretic and relaxation effects, Wein effects, Debye – Fulckenhegen effect.

**E: Molecular Spectroscopy** **10**

Time dependent perturbation theory: Harmonic – perturbation and Fermi golden rule, Einstein's coefficients of induced emission and absorption, molecular term symbols, Electronic spectra of polyatomic molecules.  $n \rightarrow \delta^*$ ,  $\delta \rightarrow \delta^*$ , CT transition, Effect of solvent, Vibronic progression, Oscillator strength, Luminescence and energy transfer processes, Mossbauer Spectroscopy, Photoelectron spectroscopy, Theory and applications to magnetic resonance spectroscopy (NMR, ESR etc).

**Course ID - PHY – P/04** **80****Practical**

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 Huckel Onager-equation.
5. Studies on the kinetics of reaction between  $K_2S_2O_8$  and KI spectrophotometrically.
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  $H_2O/C_6H_6/CH_2COOH$ .

**Semester- III****Common Paper****Course ID - IOP - T/05****A: Analytical Chemistry:** **5**

- Recapitulation of the elementary concepts of Analytical Chemistry.
- Selected analytical techniques:
  - ∅ Solvent extraction.
  - ∅ High performance liquid chromatography (Brief ideas).

**B: NMR Spectroscopy**

7

**Number of Classes**

Introduction to the techniques and Application of NMR:  $^1\text{H}$  and  $^{13}\text{C}$  NMR - principles, instrumentation; principles of decoupling, gated and inverse gated decoupling, NOE, relaxation process, selective polarization transfer, INEPT, basic two-dimensional sequence, homonuclear and heteronuclear shift correlation.

**C: Organometallic Reagents**

8

Principle, preparations, properties and application of organometallic compounds of transition elements – Cu, Pd, Ni, Fe, Co, Rh, Ru, Cr and Ti in organic synthesis and in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerisation and polymerization), structure and mechanistic aspects, Davies rule, catalytic nucleophilic addition and substitution reaction, coupling reaction – Heck, Stille, Suzuki coupling, Sonogashia, Buchwald-Hartwig, Ziegler Natta reaction, Walker Process, Olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, functional organometallic compounds, pi-acid metal complexes, activation of small molecules by coordination.

**D: Reagents in organic synthesis**

5

Use of following reagents in organic synthesis and functional group transformations – complex metal hydrides, Gilman's reagent, lithium dimethyl cuprate, LDA, DCC, 1,3 - Dithane (reactivity umpolung). Merrifield resin, Peterson's synthesis, Lawesson's reagent. Wilkinson's catalyst, Baker yeast., hypervalent organo iodines (introduction) and reagents of non transition metals – Zn, Cd, Sm and In.

**E: Advanced Quantum Chemistry**

7

Many electron treatment, Pure-spin states, Slates-Condon rules, Hartree-Fock theory, Hartree-Fock-Roothaan method.

**F: Group theoretical representation and spectroscopy**

4

Reducible and irreducible representations, classes and characters, Great Orthogonality and related theorems.

**G: Polymer Chemistry**

4

Theory of polymers solutions, entropy and Flory-Huggins theory, Commercial polymer and bio-medical applications, Polyethylene, polyvinyl chloride, polyamides, polyester, phenolic resins epoxy resins and silicone polymers, Functional polymers-Fire retarding polymers and electrically conducting polymers.

**Number of Classes****Course ID - PHY – T/06****A: Statistical Thermodynamics****20**

Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translational, rotational vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions, Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions,

**B: X-ray diffraction and Solid State****10**

Bragg-Miller indices, X-ray structural analysis of crystals, identification of unit cells, structure of simple lattices and X-ray intensities, Defects in solids: point, line and plane defects, Determination of equilibrium concentration of Schottky and Frenkel defects, F-centres/color-centres in ionic crystals, Band theory of solids, Semiconductors (extrinsic and intrinsic), hopping semi-conductors, rectifiers, transistors, Super conductivity, Organic conducting solids, solid state reactions.

**C: Biophysical Chemistry****10**

Structure of Biomolecules: protein, nucleic acid, carbohydrates and lipids, Membrane structure, Biomolecular complexes : protein-ligand, enzyme- substrate and drug-DNA complexes with examples. Techniques for study of biomolecular structure and function: Fluorescence and CD, surface tension, surface pressure area, etc measurements.

**Course ID - PHY – P/07****80****Practical**

1. Determination of CMC and micellization parameters of an ionic surfactant conductometrically.
2. Studies on the effect of ionic strength on the micellization of SDS.
3. Spectral studies on Py - I<sub>2</sub> charge transfer complex.
4. Determination of the activation energy of the reaction between K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> and KI.
5. Determination of the activation energy of the reaction between KBrO<sub>3</sub> and KBr.
6. Determination of isoelectric point of gelation viscometrically
7. Determination of E<sup>o</sup> of Ag<sup>+</sup> /Ag electrode and solubility product of AgCl.
8. Estimation of Cl<sup>-</sup>, Br<sup>-</sup> and I<sup>-</sup> in a mixture potentiometrically.
9. Determination of coordination number of Ag<sup>+</sup> ion in Ag-ammine complex potentiometrically.
10. Determination of composition of Fe<sup>2+</sup> - salicylate complex by Job's method.

**Semester- IV****Number of Classes****Course ID - PHY – T/08****A: Polymer Chemistry****10**

Plastics, elastomers and fibers, Compounding, Processing techniques; models of polymers; viscoelasticity, Biomedical polymers-contact lens, dental polymers, artificial heart kidney, skin and blood cells, Organic and Inorganic polymers.

**B: Advanced Electrochemistry****5**

Structure of electrified interfaces, Guoy-Chapman, Stern, Tobin etc. models; overpotential, exchange current density, Butler-Volmer equation, Tafel plot.

Quantum aspect of charge transfer at the electrode – solution interfaces, Electrocapillarity (EC), nature of EC curves, Lipmann equation, Electrical double layer theory. Electrochemistry at semiconductor interfaces; Electrocatalysis, Photoelectrochemistry, Theory and application of polarography, cyclic-voltammetry. Bioelectrochemistry; Introduction to corrosion, forms of corrosion, corrosion monitoring and prevention methods,

**C: Chemical Kinetics****5**

Theories of unimolecular reactions: Lindemann, Hinshelwood, Rice-Ramsperger-Kassel (RRK) and Rice-Ramsperger-Kassel-Marcus (RRKM) theories.

**D: Advanced Quantum Chemistry****10**

Basis functions, Electron correlation, Configuration interaction, Born-Oppenheimer approximation, Introduction to Density functional theory.

**E: Group theoretical representation and spectroscopy****10**

Projection operator, Direct product representation Applications: SALC, Spectroscopic selection rules, Polyatomic vibration and normal modes.

**Course ID - PHY – T/09****A: Non equilibrium Thermodynamics****10**

Thermodynamic criteria for non-equilibrium process, Entropy production and entropy flow, Entropy balance equations for heat flow, chemical reactions etc., Transformations of the generalized fluxes and forces, Nonequilibrium stationary states, Generalized flux and forces, Phenomenological equations, Onsager reciprocal relations, Principle of detailed balance, Electro kinetic phenomenon, Diffusion, Electric conduction, Transport number and electrochemical cells, Irreversible thermodynamics for biological systems.

	<b>Number of Classes</b>
<b>B: Advanced Material</b>	<b>20</b>
Glasses, ceramics, composites and Nano materials. Glasy state, glass formers and modifiers, applications, ceramic structures, mechanical properties, clay products, refractories, characterization, property and application. Preparation, characterization, properties, applications of nanomaterials.	
Thin Films and Langmuir – Blagett films: Preparator techniques, chemical, MOCVD, sol-gel etc. CB films, growth technique, Properties and applications. Liquid Crystals: Mesomorphic behavior, different phases in liquid crystals order parameters, textures, twisted and chiral nematics, chiral nematics, application of liquid crystals.	
<b>C: Quantum statistical thermodynamics and nonequilibrium Statistical Mechanics:</b>	<b>10</b>
Fermi-Dirac statistics, distribution law and applications to metal, Bose Einstein statistics-distribution law and application to helium. Elementary ideas of Brownian motion, Einstein theory, relation between diffusion and mobility, Langevin equation.	
<b>Course ID - PHY – P/10:</b>	<b>80</b>

**Practical**

1. Determination of  $pK_a$  of methyl red indicator spectrophotometrically.
2. Determination of  $pK_a$  of phenolphthalein indicator spectrophotometrically.
3. Study the effect of ionic strength on the kinetics of  $K_2S_2O_8 + KI$  reaction.
4. Study on the effect of ionic strength on the kinetics of  $KBrO_3 + KBr$  reaction.
5. Study the kinetics of inversion of cane sugar polarimetrically.
6. Tensiometric study on the micellization of a nonionic surfactant.
7. Experiments on: Computer application in solving different physicochemical problems.

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