DEPARTMENT OF CHEMISTRY
UNIVERSITY OF NORTH BENGAL

Accredited by NAAC with Grade A

Enlightenment to perfection

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

New Syllabus for M. Sc. (Regular under CBCS pattern) in Chemistry with effect from 2019-2020 session

(Course Duration = Four Semester Two year)

Total Credits = 72

Theory (T) = 48 Credits Practical (P) = 12 Credits Cont. Evaluation (CE) = 12 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)			ORG/ING/ PHY-P/01	150	3	Continuing Evaluation /1 (Equal weightage)			
	ORG-T/01	50	3				50	3		
	Inorganic Chemistry (ING)									
	ING-T/01	50	3							
	Physical Chemistry (PHY)									
	PHY-T/01	50	3							
	PHY-T/02	50	3							
Marks / Credits		**200**	**12**		**150**	**3**	**50**	**3**	**400**	**18**
II	Organic Chemistry (ORG)			ORG/ING/ PHY-P/02	150	3	Continuing Evaluation /2 (Equal weightage)			
	ORG-T/02	50	3				50	3		
	Inorganic Chemistry (ING)									
	ING-T/02	50	3							
	ING-T/03	50	3							
	Physical Chemistry (PHY)									
	PHY-T/03	50	3							
Marks / Credits		**200**	**12**		**150**	**3**	**50**	**3**	**400**	**18**
III	Organic Chemistry (ORG)			ORG/ING/ PHY-P/03	150	3	Continuing Evaluation /3 (Equal weightage)			
	ORG-T/03	50	3				50	3		
	ORG-T/04	50	3							

	Inorganic Chemistry (ING)									
	ING-T/04	50	3							
	Physical Chemistry (PHY)									
	PHY-T/04	50	3							
	Marks	**200**	**12**		**150**	**3**	**50**	**3**	**400**	**18**
IV	Organic Chemistry (ORG)						Continuing Evaluation /04 (Equal weightage)			
	ORG-T/05 ORG-T/06 ORG-T/07 ORG-T/08	50 50 50 50	3 3 3 3	ORG-P/04	50	1	50	3		
	Inorganic Chemistry (ING)									
	ING-T/05 ING -T/06 ING -T/07 ING -T/08	50 50 50 50	3 3 3 3	ING -P/04	50	1				
	Physical Chemistry (PHY)									
	PHY-T/05 PHY-T/ 06 PHY -T/07 PHY -T/08	50 50 50 50	3 3 3 3	PHY -P/04	50	1				
	Project - Dissertation									
				ORG/ING/ PHY – PD/05	100	2				
	Marks	**200**	**12**		**150**	**3**	**50**	**3**	**400**	**18**
Total Marks		**800**	**48**		**500**	**10**	**400**	**14**	**1600**	**72**

ORGANIC CHEMISTRY: THEORETICAL

PAPER- ORG-T/01

1. **Aromaticity**: Benzenoid and non-benzenoid compounds-generations and reactions. (**L = 6**)
2. **Principles of Stereochemistry**: Configurational and conformational isomerism in acyclic and cyclic compounds; Stereogenecity, Stereoselectivity, Enantioselectivity and Diastereoselectivity and Asymmetric induction. (**L = 10**)
3. **Carbon Carbon Single and Double Bond Formation:** Alkylation of enolates and enamines, Conjugate addition reactions of enolates and enamines, Asymmetric aldol reaction, β-Elimination reactions, Pyrolytic *syn*eliminations, Fragmentation reactions, Alkenes from hydrazones, Alkenes from 1,2-diols, Alkenes from alkynes, The Wittig and related reactions, Alkenes from sulfones. (**L = 10**)
4. **Spectroscopy**: Structure determination of organic compounds by UV-VIS, IR, ^{1}H, ^{13}C NMR and Mass spectroscopic techniques (Part-I). (**L = 10**)

PAPER-ORG-T/02

1. Radical species; radical initiators, reactivity pattern of radicals, detection, determination and studies of reaction involving radical pathways. (**L = 14**)
2. Common named reactions and rearrangement reactions-applications in organic synthesis. (**L=8**)
3. **Organic Transformations and Reagents**: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic), chemo, regio and stereo-selective transformations. (**L = 14**)

PAPER-ORG-T/03

1. **Advanced Stereochemistry**: Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction-substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination, resolution-optical and kinetic. (**L = 14**)
2. **Nitrogen (N), Oxygen (O), Sulfur (S) containing Heterocycles**: Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatom (O, N, S). (**L = 14**)
3. **Organic Reaction Mechanism**: Organo-catalysis and asymmetric synthesis. (**L = 8**)

PAPER-ORG-T/04

1. **Photochemistry and Pericyclic Reaction**: Basic principles, Jablonski diagram, photochemistry of olefinic compounds, Cis-trans isomerisation, stereomutationPaterno-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.

Thermal and photopericyclic reactions, Selection rules and stereochemistry of electrocyclic reactions, cycloadditions, sigmatropic rearrangements, carbene addition, cheleotropic reactions. Rationalization based on Frontier M.O. approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems, Sommelet-Hauser, Cope, aza Cope and Claisen rearrangements , Ene Reaction, Wittig rearrangement, suitable examples of [(2π +2 π), (4π +2 π), (4π + 4π), (2π +2 π +2π)] and metal catalysed cycloaddition reactions

(L = 12 + 12)

2. **Natural Products**: Terpenoids (sesqui-, di- and tri-terpenoids), carbohydrates **(L = 12)**

PAPER-ORG-T/05

1. **Organometallic Chemistry**: 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, π-acid metal complexes, Activation of small molecules by coordination. **(L = 25)**
2. **Catalysis and Green Chemistry**: Green Chemistry – overview, Set of principles of green chemistry, Green synthetic methods, Solid acids and bases as catalysts, Catalytic reductions, Catalytic oxidations, Catalytic carbon–carbon bond formation, Hydrolysis, organic synthesis in aqueous media, Ionic liquid, Supercritical fluids and microwave, Solvent free organic reactions, Solid phase organic synthesis, Chemicals from renewable raw materials, Process integration and cascade catalysis. **(L = 20)**

PAPER-ORG-T-06

1. **Vitamins**: Structure determination of Vitamin A, B, C, D, E and K and their biological impact. **(L = 15)**
2. **Medicinal chemistry**: General accepts of Medicinal Chemistry, Drug action at enzymes, Drug action at receptors, Lead compound discovery strategies, QSAR, Antibacterial agents, Opium analgesic, Cimetidine, Steroids and their chemistry. **(L = 15)**
3. **Bio-organic chemistry:**Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structureand Biological functions of coenzymes A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FAD, lipoic, vitamin B. Mechanisms of reactions catalyzed by the above cofactors.

   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. **(L = 15)**

PAPER-ORG-T/07

1. **Natural products-II**: Alkaloids (pyridine and quinolone based) structure determination and chemistry. **(L = 15)**
2. **Flavonoids**: 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 and shikimic pathway. **(L = 30)**

PAPER-ORG-T/08

1. **Concepts in organic synthesis**: Retrosynthesis, Disconnection, Synthons, Linear and convergent synthesis, Umpolung of reactivity and protection/deprotection of functional groups. **(L = 15)**

2. **Advanced spectroscopy**: Application of DEPT, 1H- ^{1}H COSY, HETCOR, TOCSY, NOESY in structure elucidation of organic compounds, drug screening, Reaction monitoring etc. q - NMR & DOSY.Modern techniques of mass spectroscopy: FAB, MIKE LCMS / MS, ES / MS, MS-MS. **(L = 15)**
3. **Compounds of non-metals:**Chemistry of Organosulphur, Organophospohorus, Organo silicon, Organoboron compounds. **(L = 15)**

ORGANIC CHEMISTRY: PRACTICAL

ORG-P/01 **60**

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).

ORG -P/02

60

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.

ORG-P / 03 **60**

Organic multi-step preparations by the use of organic reagents and purification of the products by chromatographic techniques.

Extraction of Natural products & their purification (Thin layer and Column Chromatography) and partial characterization by IR, UV and NMR.

ORG-P / 04 **40**

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.

ORG-PD/05 **60**

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

INORGANIC CHEMISTRY: THEORETICAL

Course Id: ING-T/01 **Marks: 50 Credit = 3**

A: Comparative chemistry of the Mn, Fe, Co, Ni and Cu group elements (10 Marks, 14 Hrs)
General properties of the elements, chemical reactivity and trends: their oxides, chalcogenides, oxoanions, halides, oxohalides, coordination and organometallic compounds highlighting structure (molecular/electronic), reactivity, spectral, magnetic properties and applications like catalytic, medicinal, etc.

B: Comparative chemistry of f-blocks elements (10 Marks, 14 Hrs)
General properties of the elements, Chemical reactivity: Trend in ionization energies and electrode potentials and their relationship to oxidation states, magnetic and spectral properties. The dioxo ions- AnO_2^+ and AnO_2^{2+}, their bonding and aqueous chemistry. Lanthanide shift reagents and analytical applications like luminescence studies, probes in life/earth sciences.

C: Organometallics-I (10 Marks, 14 Hrs)
Structure and bonding of organometallic compounds of Gr-I, II, III, IV elements. 18-electron rule, metal carbonyls, nitrosyls, cabonyl hydrides, dioxygen and dinitrogen compounds.

D: Chemistry of Cluster compounds (10 Marks, 14 Hrs)
Electron deficient compounds- synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, structure and bonding in higher boranes based on Lipscomb's topological concept, Wade's rules, Borohydride anions, Organoboranes and hydroboration, Carboranes, Metalloboranes, Jemmis mno rule.

E: Nuclear Chemistry (10 Marks, 14 Hrs)
Nuclear forces, liquid drop model, shell model and Magic numbers. Nuclear spin and nuclear isomerism. Nuclear reactions-energetics, mechanism and models. Nuclear fission and nuclear fusion. Nuclear reactors and particle accelerators. Interaction of radiation with matter: Nuclear activation analyses, Charged particle activation analyses. Radiotracer methods: study of chemical reactions, nuclear medicine, isotope dilution analysis. Radioanalytical techniques: particle induced X-ray emissions, Rutherford back scattering spectrometry and hot-atom.

Course Id: ING-T/02 **Marks: 50 Credit = 3**

A: Organometallics-II (10 Marks, 14 Hrs)

Isolobal and isoelectronic analogies. Metal-metal bonding (MO approach), metal-metal single and multiple bonded compounds. Bonding in dimolybdenum and dirhenium complexes. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, caping rules. Reactions of organometallic compounds: substitution, oxidative addition, reductive elimination, migrator insertion, electrophic and nucleophic reactions.

B: Reaction mechanisms of transition metal complexes-I (10 Marks, 14 Hrs)

Classification of the reactions of complex compounds, thermodynamic and kinetic stability, 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, experimental aspects of kinetic studies using UV-VIS spectroscopy (e.g., stopped-flow method and variable temperature measurements), some important rate laws, activation parameters from the Eyring plot ($\Delta S^{\#}, \Delta H^{\#}, \Delta V^{\#}$), 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 (twist mechanisms).

C: Magnetochemistry-I (10 Marks, 14 Hrs)

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.

D: Acid-Base Chemistry (10 Marks, 14 Hrs)

Strength of acids and bases, Factors governing acid strength, solvent leveling effect, Lux-Flood concept, HSAB, HOMO-LUMO concept, effect of hard and soft acids and bases, super acids. Heterogeneous acid-base reactions: surface acidity, solid and molten acids in industrial processes.

E: **Inorganic substances in non-aqueous media** (10 Marks, 14 Hrs)

Properties of ionizing solvents: Liquid NH_3, SO_2, H_2SO_4, HF and HCN as solvents.

Course Id: ING-T/03 **Marks: 50 Credit = 3**

A: Reaction mechanisms of transition metal complexes-II (10 Marks, 14 Hrs)

Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution process, nucleophilicity parameter, etc. Two types of electron transfer processes involving either no net chemical change (self-exchange and cross reactions) or those in which there is a chemical change, kinetic aspects of an electron transfer process: the decisive role of one-electron transfer step with binary collision along with the Franck-Condon barrier. Two electron transfers: complementary and non-complementary reactions, redox reactions involving oxygen atom transfers, mechanisms of outer-sphere and inner- sphere electron transfer reactions, theory of outer sphere processes, the Marcus cross

relation, thermodymanic aspects of electron transfer reactions-correlation of CFSE and E^o values of complex compounds.

B: Redox Chemistry (10 Marks, 14 Hrs)

Standard reduction potentials, cell construction conventions and energetics (e.g., evaluation of K, ΔG^o, ΔH^o, ΔS^o), utility of Ellingham, Latimer, Frost and Pourbaux diagrams-evaluating the ease of reduction of metal oxides/sulphides, interpreting different redox events in inorganic and bioinorganic chemistry. Electrochemical behaviour of coordination compounds and Cyclic Voltammetry (preliminary idea).

C: Magnetochemistry-II (10 Marks, 14 Hrs)

Magnetic properties (of 3d series transition metals) based on the crystal field model, quenching of orbital magnetic moment by the crystal field, the quantitative relation between μ_{eff} and μ_s as well as the outlines of its derivation, spin-orbit coupling and A, E, T ground terms, applications to Co(II) complexes, anomalous magnetic moments, magnetic exchange coupling and spin cross-over phenomena, paramagnetic dimmers-examples of Cu(II), VO(IV) complexes.

D: Isopoly and heteropoly acids and their salts/Polyoxometallates (10 Marks, 14 Hrs)

Isopoly and heteropoly acids of V, Mo and W and their salts: synthesis, structures, reactions and uses. Carbide, nitride, chalcogenide and halide containing clusters. Molybdenum blue, tungsten blue, rhenium blue, platinum blue, tungsten bronze, rhenium red: Synthesis, structure, reactions and bonding. Cluster compounds of Nb, Ta, Mo and W and their application in catalysis.

E: Medicinal chemistry-I (10 Marks, 14 Hrs)

Pharmacodynamics-different types of drugs and drug targets, drug binding forces, role of enzymes. Drug-receptor interactions, mechanism of drug action, agonists, antagonists. Affinity, efficacy and potency of a drug, dose-response curves. Pharmacokinetics-drug absorption, distribution, metabolism (Phase-I and Phase-II transformations), excretion and drug formulation.

Course Id: ING-T/04 **Marks: 50 Credit = 3**

A: Analytical chemistry-I (12 Marks, 16 Hrs)

Systematic and random errors, Accuracy and precision, Ways of expressing accuracy and precision, Normal error curve and its equation, Propagation of error, Useful statistical test: test of significance, the F test, the student 't' test, the chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values, significant figures, regression analysis (least-square method for linear plots), statistics of sampling and detection limit evaluation.

B: Molecular symmetry and Group theory (14 Marks, 22 Hrs)

Symmetry elements and symmetry operations, definition of group, sub group, relation between orders of a finite group and its sub groups, conjugacy relation and classes, point symmetry group, Schonflies symbols, representation of groups by matrices, character of a representation, the great orthogonality theorem (without proof) and its importance, character tables and their use.

C: Medicinal Chemistry-II (12 Marks, 16 Hrs)

Drug design and synthesis, Molecular and quantum mechanics; Drawing chemical structures, equations, and diagrams; 3D structures; Molecular modelling and Energy Minimization; Molecular properties, Conformational analysis, Docking Procedures, De novo design, Molecular Recognition,

Receptor Based Molecular Modelling, QSAR studies, Antineoplastic agents, cardiovascular drugs, Local anti-infective dugs, Antimalarial, Antibiotics, Anticholenergic and CNS-active drugs.

D: Green Chemistry (12 Marks, 16 Hrs)

Definition, Principles of Green Chemistry, Examples and illustration, Metal ion/complexes mediated green chemical synthesis of laboratory and industrial importance. Preliminary concepts of Supramolecular chemistry.

Course Id: ING-T/05 **Marks: 50 Credit = 3**

A: Organotransition metal Chemistry-I (10 Marks, 14 Hrs)

Alkyls and aryls of transition metals, Compounds of transition metal-carbon multiple bonds and Transition metal-π-complexes.

B: Chemical bonding-I (10 Marks, 14 Hrs)

Crystal field theory- splitting of d- orbitals in electrostatic fields of different symmetry, 10Dq value, spectrochemical and nepheloxetic 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 σ- and π-bonding, comparison of VBT, CFT and MOT (Application of group theory as and when needed in the above cases).

C: Photoinorganic chemistry (10 Marks, 14 Hrs)

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-spliting of water and solar energy conversion/storage.

D: Solid State chemistry (10 Marks, 14 Hrs)

Vacancy defects in elemental solids, Schottky defects, Self-interstitial in elemental solids, Frenkel defects in ionic solids, Electronic properties and Band theory, Interstitial impurity in metals, Aliovalent impurity, Charge compensation in ionic solids, Non-stoichiometry, Colour centres, Photographic process, Phosphors.

E: Analytical chemistry-II (10 Marks, 14 Hrs)

Selected analytical techniques-I

a) Solvent extraction
b) High performance liquid chromatography (Brief ideas)
c) Ion exchange chromatography
d) Polarography, amperometry, cyclic voltammetry and controlled potential coulometry (CPC) for evaluating the 'n' value.

Course Id: ING-T/06 **Marks: 50 Credit = 3**

A: Analytical chemistry-III (20 Marks, 28 Hrs)

Selected analytical techniques-II

a) Spectrophotometry: Principles and methods, instrumentation (brief outline), isobestic points, spectrophotometric titrations, spectrophotometric determination of the stoichiometry/stability constants

of coordination compounds: Job's method of continuous variation, slope ratio, mole-ratio method and their limitations.

b) Thermal methods of analysis: TGA, DTG and DTA-Principles and methods, instrumentation (brief outline), presentation of thermal data, factors affecting the results of thermal analysis, implication of combinational TG-DTA technique and applications.

c) Radioactive methods of analysis and their applications: Neutron activation analysis, Isotopic dilution method, Reverse isotopic dilution method and Radiometric titrations.

d) Fluorimetry, nephelometry, turbidometry and atomic absorption spectroscopy: Principles and methods, instrumentation (brief outline) and applications.

B: Chemical bonding-II (10 Marks, 14 Hrs)

Analysis (with respect to position, intensity and width) and assignments of electronic absorption spectra of complex compounds [O_h and T_d systems as well as D_{4h} resulting from $O_h \rightarrow D_{4h}$ symmetry lowering]: oscillator strength, transition moment integral, vibronic fine structure, selection rules, mechanisms of breakdown of selection rules, d^1 and d^9 systems (hole formalism), Orgel diagrams, multi-electron systems (d^2-d^8), high-spin Mn(II) system: intensity and line widths, Tanabe-Sugano diagrams for various d^n (n = 2-8) systems, determination of *Dq*, *B* and *β*-parameters, ACFT and charge transfer spectra.

C: Bioinorganic chemistry-I (10 Marks, 14 Hrs)

Biometals and their pivotal role, Biological basic processes in living world: Photosystems, Transport and storage of dioxygen, Respiration, ion transport, and N_2 fixation and their insights

Nucleic Acids: RNA, DNA, base-pairing, double helical structure of DNA, Gene regulatory protein-Zinc finger protein.

D: Organotransition metal Chemistry-II (10 Marks, 14 Hrs)

Transition metal compounds with bonds to hydrogen, Organometalic catalysts: activation of small molecules by coordination, homogeneous and heterogeneous catalytic reactions and Fluxional organometallic compounds.

Course Id: ING-T/07 **Marks: 50 Credit = 3**

A: Advanced Group theory (10 Marks, 14 Hrs)

Normal mode analysis, IR, Raman active modes, feasibility of different UV transitions. Application of group theory towards IR active modes of different metal carbonyls and coordination compounds. MO formation using group theory (symmetry adapted linear combination of atomic orbitals).

B: Bioinorganic chemistry-II (10 Marks, 14 Hrs)

Electron transfer in biology:

Structure and functions of metalloproteins in electron transfer process: iron-sulfer proteins, cytochromes. Metalloenzymes of iron, copper and zinc: Ferritin, Catalase, peroxidase, tyrosinase, Superoxide dismutase, carbonic anhydrase, carboxypeptidase, urease, and cobalamin complex (Vitamin B_{12}), Metabolism and Energetics: Glycolysis and oxidative phosphorylation.

Enzyme: Enzyme kinetics and applications of metallo-enzymes in living systems. Relationship between metal complexes and their medicinal activity towards different biological concerns. Chelation therapy and their approaches to drug design.

C: Spectroscopic techniques-I (10 Marks, 14 Hrs)

Characterization of Inorganic compounds by vibrational, rotational, NMR (^{11}B, ^{31}P, ^{19}F and ^{15}N, etc) and Mössbaur Spectroscopy.

D: Molecular spectroscopy (10 Marks, 14 Hrs)

Electric dipole transitions, Einstein's treatment of absorption and emission phenomena, Probability of emission and its application to lasers, Stationary states, Transition moment integral, Correlation with experimental quantities, Intensity of electronic transitions, Oscillator strength, Selection rule for transition, Modification of selection rules, Charge transfer transition, Potential energy diagram, Franck-Condon principle, Quantum mechanical formulationof Franck-Condon principle, Crossing of potential energy surfaces, Emission spectra, Environmental effect on absorption and emission spectra.

E: **Chemistry of the missing elements and super heavy elements** (10 Marks, 14 Hrs)

General chemistry of Tc, Pm, Fr, At and elements with Atomic number 104-118.

Course Id: ING-T/08 **Marks: 50 Credit = 3**

A: Spectroscopic techniques-II (10 Marks, 14 Hrs)

Characterization of Inorganic compounds by EPR, ORD/CD, EXAFS and ESCA, XPS and UPS.

B: Crystal morphology & crystallography (10 Marks, 14 Hrs)

Important minerals and different types of silicates (mica, feldspar, perovskite, talc, LDH, zeolite): structural and physical properties. Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Radius ratio rule of ionic lattices, coordination numbers, packing efficiency of lattices. Close-packing of lattices: voids; cubic close pack, Hexagonal close pack. Solid state close packing of NaCl, ZnS, CaF_2, NiAs, Diamond lattice and CsCl, etc. Structures of spinel and inverse spinel in terms of close packing. Neutron diffraction (brief idea).

C: Inorganic supramolecular chemistry (10 Marks, 14 Hrs)

Basis terms and concepts, nature and types of supramolecular forces, self-assembly of metal atoms/coordination, metal-organic frameworks (MOFs). A preliminary learning of supramolecular forces using CCDC softwares through computers.

D: Chemistry of non-transition elements (10 Marks, 14 Hrs)

Rings, cages and cluster compounds containing B-N bonds, P-N bonds and S-N bonds

E: Chemistry of Nano-materials & Advanced functional materials (10 Marks, 14 Hrs)

Fundamental physical and chemical principles, characterization, fabrication and applications of nano-materials and inorganic functional materials.

INORGANIC CHEMISTRY: PRACTICAL

Course Id: ING-P/01 **Marks: 50 Credit = 1**

Qualitative analysis: (50 marks, 90 hrs)

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

Course Id: ING-P/02 **Marks: 50 Credit = 1**

Quantitative analysis: (50 marks, 90 hrs)

Separation and estimation of two metal ions from minerals, alloys or solutions.

Course Id: ING-P/03 **Marks: 50 Credit = 1**

Quantitative analysis: (50 marks, 90 hrs)

Separation and estimation of two metal ions from minerals, alloys or solutions.

Quantitative estimation of metal ion concentration at trace level by spectroscopic techniques (UV-Visible and Atomic absorption spectroscopy)

Course Id: ING-P/04 **Marks: 50 Credit = 1**

(50 marks, 90 hrs)

a) Synthesis of inorganic compounds/complexes and their physico-chemical characterization by different analytical and spectroscopic (SCXRD, TGA, PXRD, IR, UV-Visible, NMR, EPR, etc) and magnetic susceptibility measurements (MSB, SQUID). 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, chloropentaamino 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), pentadentate ligands and their transition metal complexes specially of Ru, Rh, Re, Pt and Pd, some air and moisture sensitive inorganic compound using Glove box.

b) Hydrothermal synthesis of single crystals of metal-organic hybrid compounds, their physico-chemical and structural characterization by different analytical as well as spectroscopic techniques, specially with single crystal X-ray diffraction studies.

c) Preparation of Nano-particles and their basic applications.

Course Id: Project **Marks: 100 Credit = 2**

(100 marks, 150 hrs)

Students have to submit a Project Dissertation and present a seminar on his/her project work. Project works have to be selected on prior consultation of the faculty members of the Inorganic Branch in different fields of Inorganic Chemistry.

PHYSICAL CHEMISTRY: THEORETICAL
SEMESTER I

COURSE: PHY/T-01
MARKS: 50
LECTURE: 60
CREDIT: 3

CONTENT:

Quantum Chemistry I L45

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. TheHydrogen atom problem and its implications.

The variational method, Eckart's theorem, Application of variational method to the Helium atom problem. Linear variational method. Huckel Method, Huckel treatment for liner conjugated hydrocarbon systems, charge density and bond order calculations.

Perturbation theory (time independent nondegenerate), Application of nondegenerate perturbation theory to the Helium atom problem. Nondegenerate perturbation theory and its application to Zeeman and anomalous Zeeman effect, nonrigid rotor, anharmonic oscillator. Degenerate perturbation technique and its application to Stark effect, ground state of hydrogen molecular ion. Time dependent perturbation theory and interaction between matter and radiation. Introduction to the method of self-consistent Field, Hartree method, Koopman's theorem.Electron spin, Antisymmetry principle, Slater determinant.

Classical Thermodynamics L15

Brief review of 1^{st}, 2^{nd} and 3^{rd} 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 activitycoefficients of non-electrolytes, Application of thermodynamics to micelles and microemulsion.

COURSE: PHY/T-02
MARKS: 50
LECTURE: 60
CREDIT: 3

CONTENTS:

Macromolecules L20

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), Biodegradable and non-biodegradable polymers, Oscillating reaction.

Chemical Kinetics L15

Rate laws, molecularity, order of reaction, extent of reaction; 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. Theories of unimolecular reactions: Lindemann, Hinshelwood, Rice-Ramsperger-Kassel (RRK) and Rice-Ramsperger- Kassel-Marcus (RRKM) theories, molecular reaction dynamics-molecular beam experiments, Chemiluminescence.

Surface Chemistry and Heterogeneous Catalysis L15

Thermodynamics at the interfaces, Electrostatic and electrokinetic phenomena, surface unsaturation, adsorption/desorption, adsorption isotherm and isobar, surface area, BET isotherm, surface energy, defects, steps, kinks, solid-liquids, solid-gas phase reactions.Development of Operando spectroscopy for heterogeneous reactions, selective examples of mechanism study by Operando. Surfaces of the nanostructures, mesopores and nanopores.Zeolites and clays. Chemical reactivity and selectivity of the nanopore surfaces.

Fundamentals of Nanoscience L10

Definition, characteristics classification, synthesis, and applications. Quantization of energy states. Structure property relationship of the nanomaterials. Potential applications of nanoscience in chemistry, biology, environment, energy conversion, electronics, magnetic, etc.

SEMESTER II

COURSE: PHY/T-03
MARKS: 50
LECTURE: 60
CREDIT: 3

CONTENT:

Computers in Chemistry L15

Fundamentals of Computers, Elements of the computer language (FORTRON, BASIC, C), Constants and variables, Operations and symbols, Expressions, Arithmatic 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 broad lengths, bond angles, dihedral angles etc. of molecules extracted form a database such as Cambridge than base.

Group Theory and Symmetry L20

Groups and their properties- the concept of groups; subgroups, classes and the related theorems; commutative (abelian) groups and cyclic groups and their examples; group multiplication tables and the rearrangement theorem. Symmetry elements and operations, products of symmetry operations, equivalent symmetry elements and equivalent atoms, symmetry in platonic solids, identification of point groups, Symmetry of C60 fullerenes, Crystallographic symmetry: 32 crystal classes, Hermann–Mauguin (HM) notations, optical activity and dipole-moment on the basis of point group symmetry; similarity transformation and the invariance of characters; block diagonalisation; direct product of matrices and their characters etc. Matrix representation of symmetry operations, characters of symmetry operations in a representation, invariance of character under similarity transformation, the row / column orthogonality of characters, reducible and irreducible representations, the "Great Orthogonality Theorem" (without derivation) and its corollaries. Quantum mechanics and group representation theory, Direct product representation, Vanishing of quantum mechanical integral, Transition probability, Selection Rules, Projection operation, symmetry adapted linear combination of atomic orbitals. Application of group theory to molecular vibrations, Normal modes, Vibrational transitions, IR and Raman Spectra and Selection rule, Application of group theory to Ligand and crystal field theory, Symmetry and chemical reactions; Woodward –Hoffmann Rule.

Colloids L10

Colloids, colloidal properties (kinetic properties, optical phenomena, coagulation), stability of colloids, sol, aerosol, gel, foam, Micelles and vesicles, microemulsion.Colloids and Interfaces. Purification and separation of colloids, osmosis, dialysis, decantation, gel filtration, preparative ultra centrifugation. Characterization of colloidal particles, CMC, Zeta potential, Tyndall effect. Use of the colloids.

Solid State Chemistry L15

Bragg-Miller indices. Unit cells. X-ray structural analysis of crystals, identification of unit cells, structure of simple lattices and X-ray intensities, Different crystal systems, Diamond structure, Zinc blende structure.Defects in solids: point, line and plane defects, Calculation of Scottky and Frenkel defects by statistical thermodynamics, F-centres/color-centres in ionic crystals, Heat capacity of solids.Band theory of solids, Reciprocal space, Brillouin zone, Semiconductors (extrinsic and intrinsic), Direct and indirect bandgaps, Density of states, hopping semi-conductors, rectifiers, transistors, Super conductivity, Organic conducting solids, solid state reactions. Applications of semiconductors in catalysis, energy conversion and environment remediation.

Semester III

COURSE: PHY/T-04
MARKS: 50
LECTURE: 60
CREDIT: 3

CONTENT:

Fundamentals of Molecular Spectroscopy L20

General introduction, nature of electromagnetic radiation, shapes & width of spectral lines, Intensity of spectral lines, Fourier transform.

Microwave Spectroscopy: Moment of Inertia and Classification of molecules, Diatomic molecule as rigid rotator, non-rigid rotator, Hyperfine Structures, Stark Effect and determination of Dipole moment, Isotopic substitution effect.

Infrared Spectroscopy: Vibrational Spectra of diatomic Molecules, Harmonic Oscillator model, Anhermonic oscillator model, Rotational Vibrational spectra of real diatomic molecules, Morse potential energy diagram, bond dissociation energy, P, Q, R branches.

Raman Spectroscopy: Introduction. Classical Theory of Raman Scattering, Q. M Picture of Raman Scattering, Characteristic parameters of Raman lines, Pure Rotation and Vibrational Raman spectra, Mutual exclusion principle, Basic Principles of a Raman spectrometer, Application of Raman Spectroscopy. Electronic Spectroscopy: Fluorescence, Phosphorescence and nonradioactiveprocesses. Theories of EPR, Mossbauer and NMR.

Fundamentals of Statistical Thermodynamics L15

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 undermined 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.

Electrochemistry L15

Ions in solution

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 – Fulkenhegen effect.

Electrode-solution interface

Structure of electrified interfaces, double layer, Quantum aspects of charge transfer at the electrode – solution interfaces, resistance, two and three electrode systems, open circuit potential.

Electrochemicalredox processes

Aqueous media: Redox potentials andconvention, potentiodynamic methods, Electrocatalysis,overpotential, exchange current density, Tafel slope, electrode kinetics, reversible, irreversible and quasireversible reactions.Theory and application of polarography, Introduction to

corrosion, forms of corrosion, corrosion monitoring and prevention methods; Photoelectrochemistry, Charge transfer at semiconductor-solution interface.
Aqueous media:Organic electrolytes, quasireference electrode, redox couple, electrochemistry in organic synthesis, stereoselective transformation, electron transfer proton coupled reactions.

Biophysical Chemistry and Spectroscopy for Biomolecules L10
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: UV-vis, IR, and Fluorescence. ORD and CD, surface tension, surface pressure area, etc. measurements.

SEMESTER IV

COURSE: PHY/T-05
MARKS: 50
LECTURE: 60
CREDIT: 3

CONTENT:

Advanced Quantum Chemistry L30
Many electron atom, Pure-spin states, Slates-Condon rules, Hartree-Fock theory, Hartree-Fock-Roothaan method. Basis functions, Electron correlation, Configuration interaction. Molecular treatment, Born-Oppenheimer approximation, Valence Bond and Molecular orbital treatment of Hydrogen Molecule. Introduction to Density Functional Theory.

Non-Equilibrium Thermodynamics L30
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. Generalization of Steady State.

COURSE: PHY/T-06
MARKS: 50
LECTURE: 60
CREDIT: 3

CONTENT:

Advanced Statistical Thermodynamics L20
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.

Noncovalent Interactions L20Noncovalent interactions, its classification. Effects of noncovalent interaction in molecular rearrangement and stability. Examples of different host and guest molecules, criteria for the formation of host-guest inclusion complexes, applications of host-guest inclusion complexes in drug delivery, sensing, and pharmaceutical chemistry.

Advanced Polymer Chemistry:L20
Plastics, elastomers and fibers, Compounding, Processing techniques; models of polymers; viscoelastricity, Biomedical polymers-contact lens, dental polymers, artificial heart kidney, skin and blood cells, Organic and Inorganic polymers. Conducting polymers, Viscoelasticity.

COURSE: PHY/T-07
MARKS: 50
LECTURE: 60
CREDIT: 3

CONTENT:

Advanced Materials Synthesis L20
Methods for chemical routes: Ligand directed synthesis, micelle and reverse micelle methods, sol-gel, template assisted synthesis, hydrothermal and solvothermal synthesis, molten-salt method, chemical etching, electrodeposition, etc. Control over growth, metals, oxides, composites, alloys, carbon and Si-based materials synthesis, properties and applications; Macromolecular frameworks.

Methods for physical routes: Epitaxial growth by PVD, CVD, MBE, ALD, PLD, MOCVD, sputtering, plasma assisted synthesis. Instrumentation of different techniques, growth condition, and reactions. Growth rate, precursors, carrier gases, substrates, lattice mismatch, buffer layer. Growth of C and Si-based materials (Si, SiC, CNT, Graphene, Fullerene, etc.).
Characterization Techniques L30
Basic theories, working principles and characterizations of the advanced materials by UV-vis (DRS), FTIR (ATR), PL, PXRD, OM, SEM, TEM, EDS, XPS, Auger, AFM, STEM, Raman, TGA, DSC, etc.
Applications L10
LSPR, SERS, catalysis, solar energy conversion, sensing, drug delivery, environmental remediation, etc.

COURSE: PHY/T-08
MARKS: 50
LECTURE: 60
CREDIT: 3

CONTENT:
Photophysical Processes and Applications

1. Electromagnetic spectrum, absorption and emission of radiation, basic law of photochemistry, quantum yield and its measurements, Franck-Condon principle, Jablonski diagram, radiatiove and non-radiative

process and their time scale, unimolecular and bimolecular process, mirror-image relationship, spin state and transition. 10

2. Molecular orbital diagram of oxygen, fluorescence and phosphorescence, electronic transitions with reference to σ-σ*, n- σ*, n-π and π-π^*, selection rule, Effect of solvent on absorption maxima, conjugate polymers and 1-D box model, Correlation of spectrum with molecular structure. 7
3. Kasha's rule and its implication,Solvents effects, solvent effects on spectrum, Excited state dipolemonent and PKa calculations, fluorescence quenching, twisted intramolecular charge transfer process. 10
4. Electron transfer and its theory, excited state intramolecular proton transfer (ESIPT) process and its kinetics, photoisomerization, and delayed fluorescence, energy transfer process (Föster and Dexter type) in between organic and inorganic materials. 8

5. Photon upconversion through triplet-triplet annihilation and its kinetics 5
6. Time correlated single photon counting (TCSPC) technique, Fluorescence anisotropy, rotational dynamics and its study with the help TCSPC. 7
7. Time resolved emission spectra (TRES) and its construction from time resolved excited state lifetime decay, determination of solvent correlation function and study of solvation dynamics, probe and microenvironment dependent on solvation dynamics. 5
8. Introduction to fluorescence correlation spectroscopy (FCS) and its application. 5

PHYSICAL CHEMISTRY: PRACTICAL

PHY/P-01/02/03 (SEMESTER I, II and III)

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.
9. Studies on alkalis hydrolysis of ethyl acetate conductometrically.
10. Determination of pK_1 and pK_2 of phosphoric acid potentiometrically.
11. Determination of pK_1 and pK_2 of phosphoric acid pH metrically.
12. Verification of Debye Huckel Onager-equation.
13. Studies on the kinetics of reaction between $K_2S_2O_8$ and KI spectrophoto-metrically.
14. Studies on the kinetics of reaction between KBr_3 and KBr titrimetrically.
15. Potentiometric estimation of Fe (II) using $K_2Cr_2O_7$.
16. Ternary phase diagram of $H_2O/C_6H_6/CH_2COOH$.
17. Determination of CMC and micellization parameters of an ionic surfactant conductometrically.
18. Determination of E^o of Ag^+/Ag electrole and solubility product of AgCl.
19. Estimation of Cl^-, Br^- and I^- in a mixture potentiometrically.
20. Determination of coordination number of Ag^+ ion in Ag-ammine complex potentiometrically.
21. Determination of composition of Fe^{2+}- salicylate complex by Job's method.

22. Determination of pK_a of methyl red indicator spectrophotometrically.
23. Determination of pK_a of phenolphthalein indicator spectrophotometrically.
24. Synthesis of fluorescent compounds and their photophysics
25. pH dependent emission properties
26. LSPR of gold nanostructures
27. Enzyme kinetics

PHY/P-04 (SEMESTER IV)

1. Study the effect of ionic strength on the kinetics of $K_2S_2O_8$ + KI reaction.
2. Study on the effect of ionic strength on the kinetics of $KBrO_3$ + KBr reaction.
3. Study the kinetics of inversion of cane sugar polarimetrically.
4. Tensiometric study on the micellization of a nonionic surfactant.
5. Experiments on: Computer application in solving different physicochemical problems.
6. Studies on the effect of ionic strength on the micellization of SDS.
7. Spectral studies on Py - I_2 charge transfer complex.

PHY/PD/05: Project-Dissertation work