New Syllabus for M. Sc (under Revised CBCS Credit Structure) in Chemistry, University of North Bengal

(Course Duration = Four Semesters/Two years, Total credit = 80, Full marks = 2000)

<table>
<tr><th rowspan="2">Course Type</th><th rowspan="2"></th><th colspan="3">Semester I</th><th colspan="3">Semester II</th><th colspan="3">Semester III</th><th colspan="3">Semester IV</th><th rowspan="2">Total Credit</th></tr>
<tr><th>Paper</th><th>Credit</th><th>Total credit</th><th>Paper</th><th>Credit</th><th>Total credit</th><th>Paper</th><th>Credit</th><th>Total credit</th><th>Paper</th><th>Credit</th><th>Total credit</th></tr>
<tr><td rowspan="6">CORE[1]</td><td rowspan="3">Theory Papers</td><td>ORG-T1</td><td>2</td><td rowspan="6">12</td><td>ORG-T2</td><td>2</td><td rowspan="6">12</td><td>ORG-T3</td><td>2</td><td rowspan="6">12</td><td rowspan="6">[2]Project</td><td rowspan="6">4</td><td rowspan="6">4</td><td rowspan="6">40</td></tr>
<tr><td>ING-T1</td><td>2</td><td>ING-T2</td><td>2</td><td>ING-T3</td><td>2</td></tr>
<tr><td>PHY-T1</td><td>2</td><td>PHY-T2</td><td>2</td><td>PHY-T3</td><td>2</td></tr>
<tr><td rowspan="3">Practical Papers</td><td>ORG-P1</td><td>2</td><td>ORG-P2</td><td>2</td><td>ORG-P3</td><td>2</td></tr>
<tr><td>ING-P1</td><td>2</td><td>ING-P2</td><td>2</td><td>ING-P3</td><td>2</td></tr>
<tr><td>PHY-P1</td><td>2</td><td>PHY-P2</td><td>2</td><td>PHY-P3</td><td>2</td></tr>
<tr><td rowspan="5">DSE[1]</td><td rowspan="5">Theory Papers</td><td>ORG-D1/
ORG-D2</td><td>2</td><td rowspan="5">6</td><td>ORG-D1/
ORG-D2</td><td>2</td><td rowspan="5">6</td><td rowspan="5">ORG-D3/
ING-D3/
PHY-D3</td><td rowspan="5">2</td><td rowspan="5">2</td><td>ORG-D4/
ING-D4/
PHY-D4</td><td>2</td><td rowspan="5">10</td><td rowspan="5">24</td></tr>
<tr><td>ING-D1/
ING-D2</td><td>2</td><td>ING-D1/
ING-D2</td><td>2</td><td>ORG-D5/
ING-D5/
PHY-D5</td><td>2</td></tr>
<tr><td rowspan="3">PHY-D1/
PHY-D2</td><td rowspan="3">2</td><td rowspan="3">PHY-D1/
PHY-D2</td><td rowspan="3">2</td><td>ORG-D6/
ING-D6/
PHY-D6</td><td>2</td></tr>
<tr><td>ORG-D7/
ING-D7/
PHY-D7</td><td>2</td></tr>
<tr><td>ORG-D8/
ING-D8/
PHY-D8</td><td>2</td></tr>
<tr><td>AEC</td><td></td><td></td><td>2</td><td>2</td><td></td><td></td><td></td><td></td><td>2</td><td>2</td><td></td><td></td><td></td><td>4</td></tr>
<tr><td>SEC</td><td></td><td></td><td></td><td></td><td></td><td>2</td><td>2</td><td></td><td></td><td></td><td></td><td>2</td><td>2</td><td>4</td></tr>
<tr><td>GE[3]</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td>GE-1/GE-2</td><td>4</td><td>4</td><td>GE-3/GE-4</td><td>4</td><td>4</td><td>8</td></tr>
<tr><td></td><td></td><td colspan="2"></td><td>20</td><td colspan="2"></td><td>20</td><td colspan="2"></td><td>20</td><td colspan="2"></td><td>20</td><td>80</td></tr>
</table>

[1]Theoretical core and DSE courses have the marks distribution: Theory = 40 & continuous evaluation = 10. [2]For Project the marks distribution is: Experimental works = 75 and presentation = 25. Students have to choose any one of the DSE courses/papers listed in bunches under respective semesters. [3]Students have to choose any one of the GE papers as listed above. GE-1, GE-2, GE-3 and GE-4 stand for '*Environmental Chemistry & Waste Management*', '*Instrumental Methods of Chemical Analysis*', '*Smart Molecules & Materials*' and '*Bio-molecular Chemistry*', respectively. In any GE papers minimum uptake of students is 10 or more than 10 and the maximum uptake should not be more than 25. Marks distribution for the practical papers is: Experiments = 30, Lab. Book = 5, Regular attendance = 5 and *viva-voce* = 10. AEC & SEC courses to be formulated by respective constituted committees of the University.

ORGANIC CHEMISTRY

1st SEMESTER

Core Course Id: ORG-T1 (Theory) Marks: 50 Credit = 2

1. Carbon Carbon Bond Formation: Alkylation of enolates and enamines, Conjugate addition reactions of enolates and enamines, 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. **12L**

2. Oxidation and reduction

Oxidation of hydrocarbons, Oxidation of alcohols, Oxidation of ketones, Catalytic hydrogenation, Reduction by dissolving metals, Reduction by hydride-transfer reagents. **12L**

3. Concepts in organic synthesis: Retrosynthesis, Synthons, Linear and convergent synthesis, The disconnection approach, Chemoselectivity, Reversal of polarity, Protection/deprotection of functional groups, Stereoselectivity, Regioselectivity, One group disconnections, Two group disconnections, Reconnections. **12L**

Core Course Id: ORG-P1 (Practical) Marks: 50 Credit = 2

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, derivative preparation and complete identification use of spectroscopic techniques (IR, UV, NMR). **60L**

DSE Course Id: ORG-D1 (Theory) Marks: 50 Credit = 2

Spectroscopy of Organic compounds

Structure determination of organic compounds by UV-VIS, IR, ^{1}H, ^{13}C NMR and Mass spectroscopic techniques (Part-I). **36L**

DSE Course Id: ORG-D2 (Theory) Marks: 50 Credit = 2

Organic Photochemistry and pericyclic reactions **36L**

Organic Photochemistry: 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.

Pericyclic reactions: 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 + 2π), (4π + 2π), (4π + 4π), (2π + 2π + 2π)] and metal catalysed cyclo addition reactions.

2nd SEMESTER

Core Course Id: ORG-T2 (Theory) Marks: 50 Credit = 2

Principles of Stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds **10L**

Organic Transformations and Reagents: Functional group interconversion; common catalysts and reagents (organic, inorganic, organometallic and enzymatic), chemo, regio and stereo-selective transformations. **10L**

Some common name reactions in organic chemistry 08L

Radical species: radical initiators, reactivity pattern of radicals, detection, determination and studies of reaction involving radical pathways. **08L**

Core Course Id: ORG-P2 (Practical) Marks: 50 Credit = 2

Organic preparation involving Aldol condensation, Condensation and cyclisation reactions, Heterocyclic molecules synthesis, aromatic substitution reaction, Sandmeyer reaction and Friedel-Crafts reaction.

Quantitative analysis: Estimation of Phenol, Glucose & Sucrose, Determination of pk_a of benzoic acid.

DSE Course Id: ORG-D1 (Theory) Marks: 50 Credit = 2

Spectroscopy of Organic compounds

Structure determination of organic compounds by UV-VIS, IR, ^{1}H, ^{13}C NMR and Mass spectroscopic techniques (Part-I). **36L**

DSE Course Id: ORG-D2 (Theory) Marks: 50 Credit = 2

Organic Photochemistry and pericyclic reactions 36L

Organic Photochemistry: 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.

Pericyclic reactions: 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 [$(2\pi + 2\pi)$, $(4\pi + 2\pi)$, $(4\pi + 4\pi)$, $(2\pi + 2\pi + 2\pi)$] and metal catalysed cyclo addition reactions.

3rd SEMESTER

Core Course Id: ORG-T3 (Theory) Marks: 50 Credit = 2

Nitrogen (N), Oxygen (O), Sulfur (S) containing Heterocycles: Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatom (O, N, S). **14L**

Some rearrangement reactions **08L**

Natural Products: Terpenoids (sesqui-, di- and tri-terpenoids), carbohydrates **14L**

Core Course Id: ORG-P3 (Practical) Marks: 50 Credit = 2

Organic multi-step preparations followed by purification of the products by chromatographic techniques. Extraction of Natural products and their purification (Thin layer and Column Chromatography) and partial characterization by IR, UV and NMR spectroscopy. **60L**

DSE Course Id: ORG-D3 (Theory) Marks: 50 Credit = 2

Advanced Stereochemistry and Organocatalysis

Enantioselectivity and Diastereoselectivity and Asymmetric induction: Cram’s, Prelog’s and Felkin-Ahn model; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle.Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction-substrate, reagent and catalyst controlled reactions. **22L**

Organocatalysis **14L**

4th SEMESTER

DSE Course Id: ORG-D4 (Theory) Marks: 50 Credit = 2

Green Chemistry and Catalysis **36 L**

Green Chemistry – Overview, Set of principles of green chemistry, Green synthetic methods, Green chemistry metrics: atom economy, percent yield, reaction mass efficiency, environmental factor, etc. organic synthesis in aqueous media, Ionic liquids, Supercritical liquids, microwave assisted organic reactions, Solvent free organic reactions, Solid phase organic synthesis, Merrifield synthesis. The art of catalysis, Metal catalyzed organic reactions, characteristics of transition metals which make them suitable as catalysts, Homogeneous and heterogeneous catalysis. Catalyst and molecular activation, Catalytic reaction and the 16 electron rule, Catalysts for fine chemical synthesis, transition metal ion catalysts for organic transformations involving catalytic reductions, oxidations, carbon–carbon bond formation, hydrolysis, and their applications in epoxidation of alkenes, isomerization of unsaturated molecules, Alkene Metathesis, Oligomerisation and polymerization (Zeigler Natta polymerization), olefin oxidation (Wacker Process), Hydroformylation (oxoreaction), Fischer-Tropsch Reaction, Monsanto Acetic Acid Process, and ReppeCarbonylation.

DSE Course Id: ORG-D5 (Theory) Marks: 50 Credit = 2

Chemistry of non-metal compounds: Chemistry of Organosulphur, Organophospohorus, Organosilicon and Organoboron compounds. **16L**

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. **20L**

DSE Course Id: ORG-D6 (Theory) Marks: 50 Credit = 2

Medicinal Chemistry and nucleic acids

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. **20L**

***Nucleic acids*:** Component of nucleic acid: Nucleoside and Nucleotide, Chemical structure of Nucleotide-connectivity with sugar and phosphate group, Nomenclature and isomerism: abridged structure and formula, Chemical reactions of nucleotide and nucleoside, Enzymatic degradation of nucleic acid, Primary structure determination of nucleic acid, Chemical synthesis of nucleosides and oligonucleotides; Biosynthesis of nucleotides and folic acids; Replication, transcription, protein biosynthesis, Peptide-nucleic acid synthesis, Covalent interactions of nucleic acids with small molecules, Structural features of DNA and RNA. **16L**

DSE Course Id: ORG-D7 (Theory) Marks: 50 Credit = 2

Natural products-II:

Alkaloids (pyridine and quinolone based): structure determination and chemistry. **08L**

Flavonoids: Synthesis and reactions of coumarin and chromones; Occurrence, Nomenclature and general methods of structure determination, Isolation and synthesis of apigenin, Luteolin, Quercetin, MyrcetinQuercetin 3-glucoside, Vitexin, Diadzein, Butulin , Aureusin , Cyanidin-7-arabinoside, Cyanidin, Hirsutidin, Biosynthesis of flavonoids-acetate and shikimic pathway. **10L**

Bioorganic Chemistry

Vitamins:

Structure determination of Vitamin A, B, C, D, E and K and their biological impact. **08L**

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. **10L**

DSE Course Id: ORG-D8 (Theory) Marks: 50 Credit = 2

Advanced Spectroscopy **36L**

Application of 1D NMR and 2D NMR spectroscopy (DEPT, 1H- ^{1}H COSY, HETCOR, HMQC, HMBC, TOCSY, NOESY, q-NMR & DOSY) in structure elucidation of organic compounds, drug screening and reaction monitoring.

Mass spectrometry: Ionization methods (EI, CI, FAB, ESI, APCI and MALDI), General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens; α-, β-, allylic and benzylic cleavage; McLafferty rearrangement, retro Diels-Alder reaction, ortho effect, etc.

Modern techniques of mass spectroscopy: MIKE, LCMS, LC MS/MS, ES/MS, MS-MS.

INORGANIC CHEMISTRY

1st SEMESTER

Core Course Id: ING-T1 (Theory) Marks: 50 Credit = 2

Coordination Chemistry-I **10L**

Crystal field theory: splitting of *d*-orbitals in electrostatic fields of different symmetry (O_h, T_d, D_{4h} and C_{4V}), 10Dq value: Experimental and theoretical determination, Spectrochemical and nepheloxetic series, Structural, kinetic and thermodynamic effects of CF splitting, Tetragonal distortion and Jahn-Teller effects, 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, ACFT and ligand field theory, MOT for bonding in metal complexes with σ- and π-bonds.

Chemistry of f-blocks elements **10L**

Rare!, Abundance, Extraction of f-block elements, General physico-chemical properties, Chemical reactivity: Trend in ionization energies, radius and electrode potentials and their relationship to oxidation states, magnetic and spectral properties. Coordination compounds of the f-block elements, 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.

Organometallics –I **10L**

Fundamentals of organometallic chemistry, Stability-18-electron rule, metal carbonyls, nitrosyls, carbonyl hydrides, dioxygen, and dinitrogen compounds. Structure, bonding, and reactivity of organometallic compounds of Gr-I, II, III, IV elements.

Chemistry of Cluster compounds **10L**

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. Concept of Frustrated Lewis pair and small molecules activation.

Nuclear Chemistry **10L**

Nuclear reactions, 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, Hot Atom Theory.

Core Course Id: ING-P1 (Practical) **Marks: 50 Credit = 2**

Qualitative analysis: **60L**

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

DSE Course Id: ING-D1 (Theory) **Marks: 50 Credit = 2**

Magnetochemistry-I **8L**

Magnetic properties: paramagnetism, ferro- and antiferro magnetism and diamagnetism, Pascal constants, Russell-Saunder's terms, Microstates: Equivalent and non-equivalent multi-electron systems, Hund's Rule, Spin-orbit coupling constant, Lande interval rule, Determination of magnetic susceptibility: Gouy's balance and Evan's method.

Photoinorganic Chemistry **8L**

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.

Organometallics-II **8L**

Isolobal and isoelectronic analogies in the context of general chemistry. Metal-metal bonding (MO approach), metal-metal single and multiply 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. General synthesis of metal carbonyl clusters and their properties.

Non-aqueous Solvents and Green Chemistry **8L**

Types of solvents and their general characteristics, Properties of ionizing solvents: Liquid NH_3, SO_2, H_2SO_4, HF and HCN as solvents.

Definition, Importance, Principles of Green Chemistry, Examples and illustration, Metal ion/complexes mediated green chemical synthesis of laboratory and industrial important reagents/products.

Acid-Base Chemistry **8L**

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.

DSE Course Id: ING-D2 (Theory) **Marks: 50 Credit = 2**

Magnetochemistry-II **8L**

Thermal energy and magnetic properties, Currie equation, Curie-Weiss law, 1^{st} order Zeeman effect, Magnetic properties of first transition series metal ions, lanthanides and actinides, orbital contribution and quenching of orbital magnetic moment by the crystal field, quantitative relation between μ_{eff} and μ_s and its derivation, Spin-Orbit coupling and A, E, T ground terms, Spin pairing and cross-over region, 1^{st} order Zeeman effect and 2^{nd} order Zeeman effect, Temperature independent paramagnetism (TIP), Orbital reduction factor.

Metallo-thereuptic approach in Bioinorganic Chemistry **8L**

- Rational design of metal complexes and their medicinal activity towards different biological concerns; Chelation therapy and their approaches to drug design.
- Interaction of metal complexes with DNA.
- Enzyme kinetics and applications of metallo-enzymes in living systems.

Bio-inspired Catalysis for C-H bond activation **8L**

Synthetic High-valent metal complexes with 3d-transition metals in the context of monooxygenase, dioxygenase, and halogenaseenzymes: Structure, bonding, and reactivity towards C-H bond functionalization.

Chemistry of Non-Transition Elements **8L**

Synthesis, Properties, Structure and Bonding of: Carbon, Nitrogen, Phosphorous, Oxygen, Sulfur, Halogens, Pseudo-halogen, and Inter-halogen; Rings, cages and cluster compounds containing B-N bonds, P-N bonds and S-N bonds.

Intensity of absorption and emission spectra **8L**

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.

2nd SEMESTER

Core Course Id: ING-T2 (Theory) **Marks: 50 Credit = 2**

Coordination Chemistry-II **8L**

Assignments of electronic absorption spectra of coordination compounds, 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, Charge transfer spectra, Brief introduction to Angular Overlap Model.

Reaction mechanisms of Coordination Compounds **12L**

Classification of the reactions of coordination 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). Mechanism of isomerization reaction – linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization. Substitution reactions in square planar complexes, Trans effect, mechanism of the substitution process, nucleophilicity parameter, etc. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Frank-condon principle (non-mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), redox catalysed substitution reactions.

Organometallics-III **8L**

Advanced organometallic chemistry: fundamental basics of C-H activation, different mechanistic aspects: sigma complex, agostic complex, Investigation of reaction mechanism through Hammett study.

Redox Chemistry **8L**

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 redox rich coordination compounds, Potentiometry, polarography, Liner sweep voltammetry and Cyclic Voltammetry, Proton-coupled electron transfer (PCET), Redox-induced electron transfer (RIET), Electrocatalysis.

Defects in Inorganic Compounds **10L**

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. Inorganic Materials of Industrial Importance: Availability, forms, structure and modifications of alumina, silicates, clays, mica, carbon, zeolites.

Core Course Id: ING-P2 (Practical) **Marks: 50 Credit = 2**

Quantitative analysis: **60 L**

Separation and quantitative estimation of metal ion concentration (from minerals, alloys, commercially available milk powder), determination of phosphoric acid in commercially available soft drinks, sulfur and phosphorous in fertilizers and pesticides, hardness of tap water, etc., by complexometric titration, gravimetry and spectroscopic techniques (UV-Visible and Atomic absorption spectroscopy at trace level).

DSE Course Id: ING-D1 (Theory) **Marks: 50 Credit = 2**

Magnetochemistry-I **8L**

Magnetic properties: paramagnetism, ferro- and antiferro magnetism and diamagnetism, Pascal constants, Russell-Saunder's terms, Microstates: Equivalent and non-equivalent multi-electron systems, Hund's Rule, Spin-orbit coupling constant, Lande interval rule, Determination of magnetic susceptibility: Gouy's balance and Evan's method.

Photoinorganic Chemistry **8L**

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.

Organometallics-II **8L**

Isolobal and isoelectronic analogies in the context of general chemistry. Metal-metal bonding (MO approach), metal-metal single and multiply 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. General synthesis of metal carbonyl clusters and their properties.

Non-aqueous Solvents and Green Chemistry **8L**

Types of solvents and their general characteristics, Properties of ionizing solvents: Liquid NH_3, SO_2, H_2SO_4, HF and HCN as solvents.

Definition, Importance, Principles of Green Chemistry, Examples and illustration, Metal ion/complexes mediated green chemical synthesis of laboratory and industrial important reagents/products.

Acid-Base Chemistry **8L**

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.

<u>DSE Course Id: ING-D2 (Theory) Marks: 50 Credit = 2</u>

Magnetochemistry-II **8L**

Thermal energy and magnetic properties, Currie equation, Curie-Weiss law, 1st order Zeeman effect, Magnetic properties of first transition series metal ions, lanthanides and actinides, orbital contribution and quenching of orbital magnetic moment by the crystal field, quantitative relation between μ_{eff} and μ_s and its derivation, Spin-Orbit coupling and A, E, T ground terms, Spin pairing and cross-over region, 1st order Zeeman effect and 2nd order Zeeman effect, Temperature independent paramagnetism (TIP), Orbital reduction factor.

Metallo-thereuptic approach in Bioinorganic Chemistry **8L**

- Rational design of metal complexes and their medicinal activity towards different biological concerns; Chelation therapy and their approaches to drug design.
- Interaction of metal complexes with DNA.
- Enzyme kinetics and applications of metallo-enzymes in living systems.

Bio-inspired Catalysis for C-H bond activation **8L**

Synthetic High-valent metal complexes with 3d-transition metals in the context of monooxygenase, dioxygenase, and halogenaseenzymes: Structure, bonding, and reactivity towards C-H bond functionalization.

Chemistry of Non-Transition Elements **8L**

Synthesis, Properties, Structure and Bonding of: Carbon, Nitrogen, Phosphorous, Oxygen, Sulfur, Halogens, Pseudo-halogen, and Inter-halogen; Rings, cages and cluster compounds containing B-N bonds, P-N bonds and S-N bonds.

Intensity of absorption and emission spectra **8L**

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.

3rd SEMESTER

Core Course Id: ING-T3 (Theory) **Marks: 50 Credit = 2**

Comparative chemistry of the Ni and Cu group elements **8L**

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 and magnetic properties.

Bioinorganic Chemistry **10L**

Elements of life: Evolution in biological systems and roles of metal ions.

Fundamental Biological Processes: Photosynthesis, Respiration and Nitrogen Fixation

Metallo-proteins for dioxygen transport/storage: Working Principle, Structural Perspectives, Functionalities (hemoglobin, myoglobin, hemerythrin and hemocyanin).

Photosynthesis: Chlorophyll, PS-I, PS-II, Z-scheme, photosynthetic electron transport chain, Oxygen evolving complex.

Nitrogen fixation: N_2 cycle, Nitrogenase enzyme: Principle, Structure and Function

Transport across biological membranes: Ionophores; Na^+-K^+-ATPase.

Cobalamins including vitamin and coenzyme B12.

Metal dependent disease: Wilson's disease, Alzheimer disease, Minemata disease, ItaiItai disease, *etc*. Toxic effects of metal ions, detoxification by chelation therapy; Metallo-therapeutics.

Molecular Symmetry and Group theory in the context of Inorganic Chemistry **10L**

Symmetry elements and symmetry operations, point group symmetry of coordination complexes and simple molecules, Schonflies symbols, Symmetry and chirality of inorganic complexes, representation of groups by matrices, the character of a representation, the great orthogonality theorem (without proof), and its importance, character tables, irreducible representation, reducible representation, Mulliken Symbols.

Supramolecular Chemistry **10L**

Basic concept and principles of Supramolecular Chemistry: Terminology and Definition, Nature of supramolecular interactions: Ion-pairing, Ion-Dipole and Dipole-Dipole interactions; Hydrogen bonding; Cation-π, Anion-π, π-π interactions, Halogen-π interaction and Van der Waal forces., Host-guest interaction, Molecular recognition and Self-assembly.

Quantum mechanical approach on transition probabilities **10L**

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 formulation of Franck-Condon principle, Crossing of potential energy surfaces, Emission spectra, Environmental effect on absorption and emission spectra.

Core Course Id: ING-P3 (Practical) **Marks: 50 Credit = 2**

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: **60L**

- Stannic iodide, bis(acetylacetonato)oxovanadium(IV), $[VO(acac)_2]$ and metal acetylacetonates, Salen and $[Fe_2(\mu\text{-}O)(salen)_2]$, *cis*- and *trans*-dichlorobis(ethylenediamine) cobalt(III) chloride, *ortho*-and *para*-hydroxy mercury(II) chloride, *cis*-and *trans*-bis(glycinato)copper(II), oxido-acetato-bridged trinuclear manganese clusters, Pentadentate ligands and their transition metal complexes specially of Ru, Rh, Re, Pt and Pd, etc.
- Synthesis of metal-organic hybrid compounds by solvothermal technique, their physicochemical and structural characterization by different analytical techniques, viz., single crystal X-ray diffraction studies, etc.
- Preparation and characterization of nano-particles and nano-composites.

DSE Course Id: ING-D3 (Theory) **Marks: 50 Credit = 2**

Magnetochemistry-III **10L**

Van Vleck equation and multiplet width, magnetic anisotropies: crystalline anisotropy and molecular anisotropy, anomalous magnetic moments, Antiferromagnetism: types and exchange pathways, Sign of J and cooperative phenomenon, Bleaney-Bowers equation, Ferromagnetism: Magnetic domains, magnetic sub-lattice, canting and weak ferromagnetism, Correlation between magnetic and structural properties.

Metallo-supramolecular Chemistry **8L**

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.

Polyoxometallates and their application **8L**

Isopoly and heteropoly acids of V, Mo, and W and their salts: synthesis, structures, reactions and uses. 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.

Fluxional compounds **8L**

Synthesis, Electronic structure and Rearrangement of some selective fluxional organometallic compounds. Mechanistic studies, Isotopic labeling, Determination of fluxionality by advanced spectroscopic techniques.

Medicinal Chemistry **10L**

Pharmacokinetics- drug absorption, distribution, metabolism, excretion, drug formulation and others; 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, Pharmacophore, QSAR.

4th SEMESTER

DSE Course Id: ING-D4 (Theory) **Marks: 50 Credit = 2**

Structural Methods in Inorganic Chemistry-I:

Vibrational spectroscopy **12L**

Vibrational motion and energies, number of vibrational modes, anharmonicity, absorption in infrared, FT spectrometers, effects of phase on spectra, vibrational spectra and symmetry, selection rules, Raman spectra and selection rules, polarized and depolarized Raman lines, resonance Raman spectroscopy, rotational fine structure in gas phase IR, Non-resonance overtones and difference bands. Application of Raman and Infrared spectra to elucidate inorganic structures, bond strength frequency shift relations, changes in spectra of donor molecules on coordination.

EPR Spectroscopy **12L**

Basic principle, presentation of spectra, Hyperfine splitting (isotropic systems), the *g* value and the factors affecting its value, anisotropic effects (the *g* value and the hyperfine couplings), interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer’s degeneracy), Shift operators and the second order effect, Electron-electron interactions, spin polarization mechanism and McConnell's relations, structural applications to transition metal complexes.

ORD/CD **8L**

Basic Principles of ORD and CD techniques, ORD and Cotton effect, Faraday and Kerr effects; Applications in determining absolute configuration of metal complexes. Applications of CD and MCD, stereoselective and stereospecific effects.

Spectrophotometry **6L**

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.

DSE Course Id: ING-D5 (Theory) **Marks: 50 Credit = 2**

Structural Methods in Inorganic Chemistry-II:

NMR spectroscopy **14L**

Application of chemical shifts, signal intensities and spin-spin coupling to elucidate structures of inorganic compounds with NMR active nuclei like ^{11}B, ^{31}P, ^{19}F and ^{15}N, etc. ^{1}H NMR spectra of coordination compounds of paramagnetic metal ions, dipolar and contact shifts, magnetic susceptibility and resonance shift. NQR spectroscopy: Principle, nuclear quadruple coupling constants, structural information from NQR spectra.

Mössbauer spectroscopy **8L**

Doppler shift and recoil energy, isomer shift and its interpretation, quadrupole interactions, effect of magnetic field on Mossbauer spectra, applications to iron and tin compounds, etc. Partial quadrupole splitting and geometry of the complexes.

Photoelectron spectroscopy **14L**

Photoexcitation and photoionization, core level (XPS, ESCA) and valence level (UPS) photoelectron spectroscopy, chemical shift, detection of atoms in molecules and differentiation of the same element in different environments from XPS, information about the nature of molecular orbital from UPS. EXAF theory- single scattering (SS) and multi scattering (MS) theory, GNXAS approach and its application to inorganic and biological systems.

DSE Course Id: ING-D6 (Theory) Marks: 50 Credit = 2

Advanced Bioinorganic Chemistry and Coordination-driven Smart Materials 36L

Part-A

- Structural/functional models of some bio-essential metallo-proteins: Metal ions transport and storage proteins: ferritin, transferin, ceruloplasmin. Hydrolytic enzymes: carbonic anhydrase, carboxy peptidase, urease, alkaline phosphatase;Bioenergetic principle and role of ATP.
- Electron transport proteins: Cytochromes, Fe–S proteins.
- Metalloproteinscatalyzing oxygen atom transfer reactions: Iron systems such as cytochrome P-450, methane monooxygenase, catechol and other dioxygenases, etc.; Molybdenum systems such as xanthine oxidase, sulphite oxidase, nitrate reductase, etc. Protective metalloenzymes such as superoxide dismutase, catalase and peroxidase.
- Oxygen Evolving Complex (OEC); Hydrogen Evolution Reaction (Hydrogenase).
- Bio-engineering of Modelled Coordination Compounds with licensed CSD software and experimental analysis with observation.

Part-B

- Structural and photonics properties of coordination-driven functional switch.
- Synthesis, structure and functional properties of coordination-driven synthetic bio-minerals.
- Bio-inspired metallo-catalysts for biological oxidative coupling reactions.
- Crystal engineering and Self-assembly of metallo-supramolecular aggregates and diversity: Learning and understanding with crystallographic softwares like Mercury, Diamond.
- Coordination-driven nano-materials and composite materials for heterogeneous catalysis, charge transport phenomenon, green and clean energy and others.
- Design of synthetic analogues for the active cores of metallo-proteins and metallo-enzymes.
- Nano-metallic Chemistry: Synthesis, characterization, and applications of nanomaterials.

DSE Course Id: ING-D7 (Theory) Marks: 50 Credit = 2

Solid State Packing of crystalline Solids 8L

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.

Crystal Morphology and X-ray Crystallography 10L

Nature of the solid-state, law of constancy of interfacial angles, the law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements, and symmetry operations, the 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.A brief discussion about neutron diffraction technique.

Chemical application of Group theory **10L**

Chemical application of group theory:Normal mode analysis, IR, Raman active modes, the 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).

Bio-inspired catalysts towards water oxidation **8L**

Artificial photosynthesis (with synthetic heme and non-heme complexes), importance, and mechanism of water oxidation (WO) in the context of artificial photosynthesis, application of molecular catalysts for WO: Different WO molecular catalysts with 3d and 4d transition metals and their mechanistic manifolds (Mechanistic understanding).

Analytical methods **6L**

Gas chromatography, HPLC, atomic absorption spectroscopy, Fluorimetry: Principles and methods, instrumentation (brief outline), and applications.

DSE Course Id: ING-D8 (Theory) Marks: 50 Credit = 2

Advanced Organometallic Chemistry **36L**

- Spectators ligands: Phosphines and carbenes, Electronic structure of transition metals, Oxidative addition involving C-X, C-H and C-C bonds, Reductive elimination, Mononuclear *versus* binuclear systems, Migratory Insertion reactions, β-hydrogen elimination reactions.
- Synthesis, Structure and stability of transition metal-alkyls and aryls complexes, Metal-carbon multiple bonds, Hapticity of ligands, Sandwich complexes, Bend sandwich complexes, Complex with alkenes and alkynes, Davis-Green-Mingos rules, Ziegler-Natta catalysis.
- Transition metal compounds with bonds to hydrogen, Organometallic catalysts: activation of small molecules by Coordination, Homogeneous and Heterogeneous catalytic reactions. Wilkinson’s catalyst, Hydroformylation oxo process, Hydrosilation, Hydroboration, Tsuji-Trost reaction, Mizoroki-Heck reaction, Suzuki-Miyaura coupling, Stille coupling, Buchwald-Hartwig amination, Olefin metathesis and Grubbs catalyst.

PHYSICAL CHEMISTRY

1st SEMESTER

Core Course Id: PHY-T1 (Theory) Marks: 50 Credit = 2

Quantum Chemistry I 30L

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

Group Theory and Symmetry 30L

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.

Core Course Id: PHY-P1 (Practical) Marks: 50 Credit = 2

1. Studies on the kinetics of iodination of acetone.
2. Determination of solubility product of PbI_2 by titrimetric method.
3. Determination of coordination number of Cu^{2+} (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 concentration of a mixed acid (mixture of a strong and a weak acid) pH metrically.
8. Studies on alkali hydrolysis of ethyl acetate conductometrically.
9. Determination of pK_1 and pK_2 of phosphoric acid potentiometrically.
10. Determination of CMC and micelization parameters of an ionic surfactant conductometrically.

DSE Course Id: PHY-D1 (Theory) Marks: 50 Credit = 2

Surface Chemistry of Colloidal and Confined Systems 30L

Colloid Chemistry: 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 ultracentrifugation. Characterization of colloidal particles, CMC, Zeta potential, Tyndall effect. Use of the colloids.

Nano Chemistry: 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.

Surface Chemistry: 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.

DSE Course Id: PHY-D2 (Theory) Marks: 50 Credit = 2

Electrochemistry 15L

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-Hückel theory, Debye-Hückel-Onsagar theory, Electrophoretic and relaxation effects, Wein effects, Debye – Falkenhagen 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.

Chemical Kinetics 15L

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.

2nd SEMESTER

Core Course Id: PHY-T2 (Theory) Marks: 50 Credit = 2

Quantum Chemistry-II 30L

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.

Solid State Chemistry 30L

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.

Core Course Id: PHY-P2 (Practical) Marks: 50 Credit = 2

1. Verification of Debye Hückel Onsager-equation.
2. Studies on the kinetics of reaction between $K_2S_2O_8$ and KI spectrophotometrically.
3. Potentiometric estimation of Fe(II) using $K_2Cr_2O_7$.
4. Ternary phase diagram of $H_2O/C_6H_6/CH_3COOH$.

5. Determination of E^o of Ag^+/Ag electrode and solubility product of AgCl.
6. Estimation of the concentration of Cl^-, Br^- and I^- ions in a mixture potentiometrically.
7. Determination of coordination number of Ag^+ ion in Ag-ammine complex potentiometrically.
8. Determination of composition of Fe^{2+}- salicylate complex by Job's method.
9. Determination of pK_a of methyl red indicator spectrophotometrically.

DSE Course Id: PHY-D1 (Theory) Marks: 50 Credit = 2

Surface Chemistry of Colloidal and Confined Systems 30L

Colloid Chemistry: 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 ultracentrifugation. Characterization of colloidal particles, CMC, Zeta potential, Tyndall effect. Use of the colloids.

Nano Chemistry: 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.

Surface Chemistry: 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.

DSE Course Id: PHY-D2 (Theory) Marks: 50 Credit = 2

Electrochemistry 15L

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-Hückel theory, Debye-Hückel-Onsagar theory, Electrophoretic and relaxation effects, Wein effects, Debye – Falkenhagen 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.

Chemical Kinetics 15L

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.

3rd SEMESTER

Core Course Id: PHY-T3 (Theory) **Marks: 50 Credit = 2**

Thermodynamics **30L**

Classical: Brief review of 1st, 2nd and 3rd 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.

Non-Equilibrium: 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.

Statistical: 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.

Fundamentals of Molecular Spectroscopy **30L**

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 nonradioactive processes. Theories of EPR, Mössbauer and NMR.

Core Course Id: PHY-P3 (Practical)   Marks: 50 Credit = 2

1. Estimation of excited state dipole moment.
2. Synthesis of fluorescent compounds and their photophysics.
3. Estimation of excited state acid dissociation constant.
4. LSPR of gold nanostructures.
5. Enzyme kinetics.
6. Study the effect of ionic strength on the kinetics of $K_2S_2O_8$ + KI reaction.
7. Study the kinetics of inversion of cane sugar polarimetrically.
8. Tensiometric study on the micellization of a non-ionic surfactant.
9. Studies on the effect of ionic strength on the micellization of SDS.
10. Spectral studies on Py - I_2 charge transfer complex.

DSE Course Id: PHY-D3 (Theory)   Marks: 50 Credit = 2

Polymer Chemistry   30L

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.
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.
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.

4^{th} SEMESTER

DSE Course Id: PHY-D4 (Theory) Marks: 50 Credit = 2

Advanced Electrochemistry

Electrochemical redox processes **30L**

Aqueous media: Redox potentials and convention, potentiodynamic methods, Electrocatalysis, over potential, 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.

Non-aqueous media: Organic electrolytes, quasireference electrode, redox couple, electrochemistry in organic synthesis, stereoselective transformation, electron transfer proton coupled reactions.

Electro kinetic phenomenon, Diffusion, Electric conduction, Transport number and electrochemical cells, Irreversible thermodynamics for biological systems. Generalization of Steady State.

DSE Course Id: PHY-D5 (Theory) Marks: 50 Credit = 2

Advanced Quantum Chemistry **30L**

Many electrons 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.

Experiments on: Computer application in solving different physicochemical problems.

DSE Course Id: PHY-D6(Theory) Marks: 50 Credit = 2

Advanced Materials: Processing & Characterization **30L**

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 of advanced materials by XRD, XPS, SEM, TEM, AFM, PL, DRS, ATR-IR, TGA, DSC, etc.

<u>DSE Course Id: PHY-D7 (Theory) Marks: 50 Credit = 2</u>

Computational Chemistry 30L

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 from a database such as Cambridge than base.

<u>DSE Course Id: PHY-D8 (Theory) Marks: 50 Credit = 2</u>

Photophysical Processes and Techniques 30L

- 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.
- 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.
- Kasha's rule and its implication, Solvents effects, solvent effects on spectrum, Excited state dipolemonent and pK_a calculations, fluorescence quenching, twisted intramolecular charge transfer process.
- 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.
- Photon upconversion through triplet-triplet annihilation and its kinetics.
- Time correlated single photon counting (TCSPC) technique, Fluorescence anisotropy, rotational dynamics and its study with the help TCSPC.
- 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.
- Introduction to fluorescence correlation spectroscopy (FCS) and its application.

GENERIC ELECTIVE COURSES

GE Course Id: GE-1 (Theory) **Marks: 100 Credit = 4**

Environmental Chemistry and Waste Management **45L**

Introduction to Environmental Chemistry: Concept and scope of environmental chemistry, the natural cycles of environment (Hydrological, Oxygen, Nitrogen, Phosphorous and Sulphur cycles). Carbon sequestration and carbon credits.

Atmosphere: Regions of the atmosphere, Reactions in atmospheric chemistry, Particles, ion and radicals in the atmosphere, stratospheric chemistry: the chemistry of ozone layer, green-house effect and Global warming, El-Nino phenomenon.

Hydrosphere: Water as a universal solvent. Concept of DO, BOD and COD. Complexation in natural water and waste-water, micro-organism in aquatic chemical reactions, Eutrophication. Water and Wastewater Pollution Control: General scheme for the treatment of water for drinking purpose. Water Treatment: UV, H_2O_2, ozonization, chemical precipitation, disinfection, adsorption, softening, desalinization / demineralization, membrane processes. Re-cycle of waste-water in process industry, treatment of sewage and reuse of water in industry and agriculture, concept of wastewater treatment plant: their importance and advantages, role in wastewater treatment.

Lithosphere: The terrestrial environment, Soil formations, Soil properties (physical/chemical), inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil. Waste and pollutants in soil, waste classification and disposal. Analysis of soil quality. Soil Pollution control. Industrial effluents and their interactions with soil components. Soil micro-organisms and their functions - degradation of pesticides and synthetic fertilizers.

Chemical Toxicology: Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical aspects of heavy metals (Hg, Cd, Pb, Cr) and metalloids (As, Se). CO, O_3, PAN, VOC, POP and carcinogens. Toxic chemicals: Pesticides and their classification and effects.

Environmental Monitoring and sampling: Concepts of environmental monitoring and its significance. Methods of physical characterization of samples, Sampling of air, water and soil: Protocol and methods of sampling, sampling devices, preservation, storage and processing of air, water and soil samples.

Principle of analytical and Instrumental methods of environmental analysis: Theory, instrumentation and applications of Titrimetry, Gravimetry Conductometry, Potentiometry, Voltammetry, Colorimetry, Thermogravimetry, Spectrophotometry, Electrophoresis and Flame photometry. Hyphenated techniques for analysis – GC-MS, HPTLC, GC-AES.

Global and Local Environmental Issues – Biodiversity loss, Climate change, Rise in Sea level. International efforts for environmental protection. Current Environmental Issues in India related to water resource projects. National Action Plan on Climate Change. Waste Management – Swachha Bharat Abhiyan.

Environmental Ethics – Environmental ethics and its principles, types of environmental ethics, Future of environmental ethics.

GE Course Id: GE-2 (Theory) Marks: 100 Credit = 4

Instrumental Methods of Chemical Analysis 45L

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.

Cyclic voltammetry, linear sweep voltammetry and coulometry: basic principles and applications. Electrochromatography: principle and applications.Polarography: principles and applications. Thermal analysis: general principles of thermal analysis. Thermogravimetric analysis (TGA): principles, instrumentation, thermogram study, applications, limitations, differential thermogram (DTG). Differential scanning calorimetry (DSC): principles, instrumentation, thermogram study, applications and limitations. Basic principles of electron microscopy—scanningelectron microscopy (SEM) and transmission electron microscopy (TEM): instrumentation, sample preparation, applications and limitations.

Principle, Instrumentation and application of UV-Vis-NIR spectroscopy, IR spectroscopy, Raman spectroscopy, Fluorescence spectroscopy, Mössbauer spectroscopy,Atomic absorption spectroscopy, ESR, X-ray crystallography, Redox chemistry and Spectro-electro chemistry,

NMR spectroscopy, Mass spectrometry, GC, HPLC, Spectroscopic investigation of some important organic and inorganic compounds.

GE Course Id: GE-3 (Theory) Marks: 100 Credit = 4

Smart Molecules and Materials 45L

Nanomaterials: Introduction to nanomaterials,physics of low-dimensional materials, 1D, 2D and 3D confinement, Density of states, Excitons, Quantum confinement effect, Zero-, One-, Two- and Three- dimensional structure, Synthesis Approach (Top down and bottom up), physical and chemical techniques for nanomaterial synthesis, Size control of metal nanomaterials and their properties:

optical, electronic, magnetic properties; surface plasmon resonance, change of bandgap; metal nanoparticles (Au, Ag and Cu), quantum dots, carbon nanotube, graphene, perovskites, nanoclusters,nano-aggregates, Supramolecular-assembled structures, Characterizations of nanomaterials with X-Ray Diffraction, Scanning Electron Microscopy, Transmission Electron Microscopy, UV-vis and Photoluminescence, Application of nanomaterials: biomedical usages (drug delivery, cancer treatment, imaging and diagnosis), catalysis, solar cells, energy conversion processes (water splitting), light emitting devices (LEDs), optical sensors, actuators, optical switches, bio-MEMS diodes and nano-wire transistors - data memory lighting and displays, filters, water purification and environmental clean-up, Future scope of Nanomaterials.

Mixed-valence chemistry: Synthesis, characterization and spectroscopic studies of mixed-valence compounds. Intervalence charge transfer and signal transfer devices. Importance of mixed-valence compounds.

Photo magnetism: Spin crossover, Light-induced Spin change, Hysteresis, Application of spin crossover complexes in future memory devices.

Solid-state fluorescent materials: Solid-state materials for versatile opto-electronic application, Solid-state brightness, LED and OLED, Aggregation Induced Emission Enhancement (AIEE) and their potential application in various fields.

Artificial Photosynthesis: Homogeneous catalysis towards water oxidation with molecular catalysts: History, different catalysts, the role of ligands, essential parameters for WO catalysts, first-row transition metal catalysts, second-row transition metal catalysts, different mechanistic pathways, intermediates required for robust and efficient catalysts.

Biopolymers and drug molecules: Basic concepts & definitions: monomer & functionality, Natural Polymers: Chemical & Physical structure, properties, source, important chemical modifications, applications of polymers such as cellulose, lignin, starch, rosin, shellac, latexes, vegetable oils and gums, proteins etc. Synthetic polymers: Manufacturing of various fractions of crude petroleum important for polymer industry, Degradation of biopolymers, Applications of Biopolymers.

Introduction to organic drug molecules for biomedical applications, Chemical structure, synthesis and property of important biologically active organic molecules, Biocompatibility, Application of organic molecules in drug delivery, curing human diseases (cancer treatment), Anticancer agents, tissue regeneration, growth and repair, impact of drug smart molecules discovery and development.

GE Course Id: GE-4 (Theory) Marks: 100 Credit = 4

Bio-molecular Chemistry 45L

Carbohydrate Chemistry: Monosaccharides, Mutarotation, Glycoside Formation, various Reactions of Monosaccharides, Oxidation Reactions of Monosaccharides, Reduction of

Monosaccharides: Osazones Formation, Synthesis and Degradation of Monosaccharides, The D Family of Aldoses, Configuration of D-(+)-Glucose (Fischer's Proof).

Disaccharides, Trisaccharides, Polysaccharides, Biologically Important Sugars, Sugars That Contain Nitrogen, Glycolipids and Glycoproteins of the Cell Surface: Cell Recognition and the Immune System, Carbohydrate Antibiotics.

Peptide and Protein Chemistry: Structure of amino acid, Physical properties of amino acid and peptides, Synthesis of amino acid, Different structures of peptides, Spectroscopic techniques to study peptide secondary structure, Basic principle of peptide synthesis, Protecting group- protection and deprotection, orthogonal protecting group, Peptide coupling agents: efficiency and drawback, Solid phase peptide synthesis, Native chemical ligation-cysteine and glutamic acid based ligation.

Chemical evolution, Urey-Miller experiment, Peptide synthesis at early earth, peptide–replication, Origins of life, Peptide-based system chemistry, Peptide responsible for different neurodegenerative disease-Alzheimer's disease and Parkinson's Disease-preliminary ideas.

Enzyme Chemistry: Nature and Bio-molecular interaction: Non-covalent, hydrophobic, binding constants and its implications, DNA organization, replication, transcription-translation, Chemical and enzymatic methods of DNA/RNA thesis, Interaction of small molecules with DNA/protein, Molecular biology-Recombinant DNA, PCR and their application. Smart biomaterials, Role of metals in biology, Analysis of biomolecules.

4th SEMESTER

CORE Course Id: Project **Marks: 100 Credit = 4**

200L

Each student has to undertake a Project under the supervision of a faculty member, 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 Department of Chemistry, NBU. They will be trained in searching research literature, experimental work and computational works as required.

===*===**