MURSHIDABAD UNIVERSITY

11, Police Reserve Road (Cantonment Area),
Berhampore, Murshidabad,West Bengal,
Pin- 742101

Website: www.msduniv.ac.in

Land (Off): -03482-295824
Phone (Off): +91-70748-13298

Email: registrar@msduniv.ac.in

Memo No.- MU(R)/1/C/500/24 **Date: 04/10/2024**

NOTIFICATION

It is notified for information of all concerned that in terms of the provision of the Murshidabad University Act, 2018, and, in existing of his powers, of the said Act, the Vice-Chancellor has, by and order dated 04.10.2024 approved the syllabi of the subject Chemistry for semester wise programme of PG Course of study under this university, as laid down in the accompanying pamphlet.

Place: Berhampore
Date: 04.10.2024

Rajib Mukherjee
Registrar
Murshidabad University

Registrar
Murshidabad University

MURSHIDABAD UNIVERSITY Estd-2021 Berhampore (W.B.)

MURSHIDABAD UNIVERSITY

CBCS Syllabus for Two Years M.Sc. in Chemistry

With effect from the session 2023-2024

DEPARTMENT OF CHEMISTRY
MURSHIDABAD UNIVERSITY
Berhampore, Murshidabad
West Bengal, India
Pin 742101

Murshidabad University Master of Science in Chemistry (2023)

Semester and Course wise credit distribution in M.Sc. Chemistry under C.B.C.S

Semester	Courses	No. of Papers	Marks	Credits
I	Core Courses	5	250	20
II	Core Courses	5	250	20
III	Core Courses DSE GE	3 1 1	250	20
IV	DSE SEC	4 1	250	20
		20	1000	80

Semester I: CC – 5 Courses

Course Code	Course Title	Course Type	Course Details	Credit	Marks	L:T:P	IA	ESE
PG-CHE-CC-101	Inorganic Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-CC-102	Physical Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-CC-103	Organic Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-CC-104(P)	Inorganic Practical	Core	Practical	4	50	0:0:2	-	50
PG-CHE-CC-105(P)	Physical + Organic Practical	Core	Practical	4	50	0:0:2	-	50

Semester II: CC- 5 Courses

Course Code	Course Title	Course Type	Course Details	Credit	Marks	L:T:P	IA	ESE
PG-CHE-CC-201	Inorganic Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-CC-202	Physical Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-CC-203	Organic Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-CC-204(P)	Inorganic + Physical Practical	Core	Practical	4	50	0:0:2	-	50
PG-CHE-CC-205(P)	Organic Practical	Core	Practical	4	50	0:0:2	-	50

Semester III: CC- 3 Courses, DSE-1, ME – 1 Course

Course Code	Course Title	Course Type	Course Details	Credit	Marks	L:T:P	IA	ESE
PG-CHE-CC-301	Inorganic Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-CC-302	Physical Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-CC-303	Organic Chemistry	Core	Theory	4	50	1:0:0	10	40
PG-CHE-DSE-304(P) [A]	Inorganic Special	DSE	Practical	4	50	0:0:2	-	50
PG-CHE-DSE-304(P) [B]	Physical Special							
PG-CHE-DSE-304(P) [C]	Organic Special							
PG-CHE-GE-313	General Chemistry	Generic Elective	Theory	4	50	1:0:0	10	40

Semester IV: DSE - 4 Courses, SEC – 1 Course

Course Code	Course Title	Course Type	Course Details	Credit	Marks	L:T:P	IA	ESE
PG-CHE-DSE-401[A]	Inorganic Special	DSE	Theory	4	50	1:0:0	10	40
PG-CHE-DSE-401[B]	Physical Special							
PG-CHE-DSE-401[C]	Organic Special							
PG-CHE-DSE-402[A]	Inorganic Special	DSE	Theory	4	50	1:0:0	10	40
PG-CHE-DSE-402[B]	Physical Special							
PG-CHE-DSE-402[C]	Organic Special							
PG-CHE-DSE-403[A]	Inorganic Special	DSE	Theory	4	50	1:0:0	10	40
PG-CHE-DSE-403[B]	Physical Special							
PG-CHE-DSE-403[C]	Organic Special							

PG-CHE-DSE-404(P) [A]	Inorganic Special	DSE	Dissertation	4	50	0:0:2	-	50
PG-CHE-DSE-404(P) [B]	Physical Special							
PG-CHE-DSE-404(P) [C]	Organic Special							
PG-CHE-SEC-405	Environmental Chemistry and Measurement	SEC	Theory	4	50	1:0:0	10	40

Total Marks: 1000, Credit: 80

CC: Core Courses, DSE: Discipline Specific Elective, GE: Generic Elective Courses, SEC: Skill Enhancement Courses.

L:T:P – Lecture Hours : Tutorial Hours : Practical Hours, IA – Internal Assessment, ESE – End Semester Examination.

[A] – Inorganic Chemistry Special, [B] – Physical Chemistry Special, [C] – Organic Chemistry Special.

SEMESTER-I

Topic name: Inorganic Chemistry (Theory)
Course Code: PG-CHE-CC-101
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Coordination Chemistry

Crystal field theory, Splitting of d orbitals in linear, triangular, tetrahedral, square planar, trigonal bipyramidal, square pyramidal, octahedral fields of similar and dissimilar ligands. Kinetic aspects of crystal field stabilization, crystal field activation energy, labile and inert complexes. Electronic spectra of transition metal complexes – determination of free ion terms of d^1 to d^9, microstates, determination of ground and all excited state terms of d^n terms in octahedral and tetrahedral fields, hole formalism, inversion and equivalence relations, selection rules for spectral transitions, d-d spectra and crystal field parameters, Nephelauxetic series, qualitative idea of Tanabe–Sugano diagrams, charge transfer spectra.

[12 lecture hours]

Unit-2: Bioinorganic Chemistry – 1

Essential elements in Biology (major and trace), beneficial and toxic elements. Bioenergetic principle and role of ATP. Transport and storage of dioxygen. Active site structure and bio-functions of O_2 – uptake proteins: hemoglobin, myoglobin, hemerythrin and hemocyanin. Model synthetic dioxygen complexes. Electron transport protein: Fe-S proteins. **[12 lecture hours]**

Unit-3: Selected topics on the chemistry of s and p block elements

Structure and bonding in higher boranes based on Lipscomb's topological concept, Wade's rules, borohydride B_nH_{n-2} anion, carboranes, metalloboranes, hydroboration reactions. Alkali metal complexes with macrocyclic ligands (crown ethers and cryptates). Aqueous and complex chemistry of beryllium and aluminium. Main group organometallic chemistry: classification, synthesis, reaction, structure and bonding, and application of typical examples. **[12 lecture hours]**

Unit-4: Nuclear chemistry

Binding energy. N/P ratios in stable and meta stable nuclei-different type of nuclear forces-liquid model shell model. Nuclear isomerism and internal conversion. Nuclear reactions-Bethes's notation, Q-value, columbic barrier, cross section, different types of nuclear reactions-projectiles capture-particle emission, spallation, fission, fusion, theories of fission, use of fission products, nuclear reactors-fissile and fertile isotopes- U_{233},U_{235},Pu_{239},Th_{232},-atomic power projects in India, stellar energy, synthetic elements-application of radio isotopes - Hot atom chemistry**.** **[12 lecture hours]**

Unit-5: Analytical chemistry-I

Errors in quantitative analyses, types of errors, handling of systematic errors. Random errors: distribution, standard deviation, confidential limits of the mean, presentation of the results, propagation of random errors. Solvent extraction: principle, distribution ratio, partition coefficient, successive extraction and

separation; effect of pH, use of different organic reagents. Chromatography: general principle, classification, mathematical relations of capacity, distribution constant, retention time; chromatogram, band broadening and column efficiency; column resolution, paper chromatography, thin layer chromatography (TLC), size-exclusion chromatography, ion-exchange chromatography, capillary electrophoresis, HPLC.

[12 lecture hours]

Topic name: Physical Chemistry (Theory)
Course Code: PG-CHE-CC-102
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Interfacial Chemistry

Curved surfaces: Young-Laplace and Kelvin equations. Adsorption of solids: BET equation. Micelles, reverse micelles; micellization equilibrium; thermodynamics of micellization; micro-and macro-emulsions.

[12 lecture hours]

Unit-2: Atomic Structure

Zeeman effect, fine structure, spin-orbit interaction, effect of high magnetic field, Lande g factor, Atomic (and molecular) terms. **[10 lecture hours]**

Unit-3: Quantum Mechanics 1

Postulates and their analysis. Properties of operators and commutators. Equation of motion. Stationary states, Quantization Schemes, Ehrenfest's theorems, some properties of one-dimensional systems, Barrier problems and tunneling. **[14 lecture hours]**

Unit-4: Kinetics 1

Fast reactions, Oscillatory reactions, Autocatalysis. Electrode kinetics: Nernst, Butler-Volmer and Tafel equations. **[10 lecture hours]**

Unit-5: Polymer Chemistry

Classification of polymers, Kinetics of polymerization, Molecular weight of polymer and its determination, Some specific methods for molecular weight determination of biopolymers-gel filtration, SDS-PAGE for proteins, Agarose gel method for nucleic acids. Thermodynamics of polymer solution: Polymer conformation. **[14 lecture hours]**

Topic name: Organic Chemistry (Theory)
Course Code: PG-CHE-CC-103
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit 1: Stereochemistry-1:
Winstein-Holness equation, Curtin-Hammett principle; Conformational analysis of cyclohexane, cyclohexene, decalin and their derivatives; 6,6; 6,5-fused bicyclic compounds perhydro anthracene, perhydro phenanthrene; etc., Addition Reactions to Carbonyl Compounds: Cram's rule, Felkin-Anh, Cieplak and Zimmerman-Traxler Models. Effects of conformation on reactivity in cyclic and acyclic systems.

[12 lecture hours]

Unit-2: Structure-Activity Relationship:
MO treatment of acyclic and cyclic conjugated systems; Huckel's rule and concept of aromaticty, annulenes, heteroannulenes, fullerenes (C60), alternant and non-alternant hydrocarbons, anti-aromaticity, pseudo-aromaticity, homo-aromaticity; graphical methods-Frost diagram. Huckel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene, Walsh orbitals of cyclopropane and cyclobutane, Linear Free Energy Relationship for substituent effect: Hammett equation and its modifications. **[12 lecture hours]**

Unit-3: Pericyclic Reactions:
Pericyclic Reaction: Introduction, classification and stereochemical modes, selection rules of electrocyclic reactions, 2-component cycloadditions and sigmatropic rearrangements. Rationalization based on PMO and FMO approach, correlation diagrams, Dewer-Zimmermann approach, Mobius and Huckel systems. Fluxional tautomerism. Sommelet-Hauser, Cope and Claisen rearrangements, Ene reaction, Wittig rearrangement. Cheletropic reactions involving neutral molecules and reactive species. **[12 lecture hours]**

Unit-4: NMR Spectroscopy 1
Principle, instrumentation and different techniques (CW & FT) of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant (J), spin decoupling, spin tickling, classification of A_2, AB, AX, AMX, ABX, AMX, ABC, A_2B_2 in proton NMR. Introduction to ^{13}C-NMR spectroscopy, principles of decoupling, gated and inverse gated decoupling techniques, NOE, relaxation processes, problems on NOE, nuclei with negative NOE. Application of NMR spectroscopy and other spectroscopical techniques to simple structural and mechanistic problems. **[15 lecture hours]**

Unit–5: Natural Products I (Terpenoids)
Terpenoids: Isoprene rule, general methods of isolation, structure elucidation(by chemical and spectroscopic methods), and synthesis of some representative members of mono and sesquiterpenes. Biogenesis and biosynthesis of mono-, sesqui- and di-terpenoids. **[9 lecture hours]**

Topic name: Inorganic Chemistry (Practical)
Course Code: PG-CHE-CC-104(P)
(50 marks)
120 Practical hours 4 Credits

Quantitative analysis

1. Gravimetric estimation of Zn(II) as $Zn(NH_4)(PO_4)$
2. Gravimetric estimation of Cu(II) as CuSCN
3. Gravimetric estimation of Ni(II) as $Ni(DMGH)_2$
4. Volumetric estimation of Mn(II)/Fe(III)
5. Volumetric estimation of Cu(II)/Cr(VI)

Synthesis and Characterization of inorganic compounds

1. Reinecke's salt, $NH_4[Cr(NCS)_4(NH_3)_2]$
2. $[Cu(en)_2(H_2O)_2]SO_4$
3. $[Ni(en)_2]Cl_2$
4. $K_3[Cr(ox)_3]$
5. Chrome alum $[K_2SO_4,Cr_2(SO_4)_3,24H_2O]$

Topic name: Physical & Organic Chemistry (Practical)
Course Code: PG-CHE-CC-105(P)
(50 marks)
120 Practical hours 4 Credits

Physical Chemistry Practical

1. To determine the adsorption isotherms of acetic acid from aqueous solution and I_2 from alcoholic solution by charcoal.
2. To investigate the adsorption of oxalic acid from aqueous solution by activated charcoal and to examine the validity of Freundlich & Langmuir's adsorption isotherms.
3. To determine the dissociation constant (Ka) of Methyl red using UV-visible absorption spectrophotometer.
4. To find surface tension/interfacial tension between two immiscible liquids.

Organic Chemistry Practical

Identification of single organic liquid with one or more functional groups.

SEMESTER-II

Topic name: Inorganic Chemistry (Theory)
Course Code: PG-CHE-CC-201
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Chemical Bonding

Different types of bondings including weak interactions; Valence bond and molecular orbital theories – comparative account; Group orbitals in molecular orbital approach; Molecular orbital description of varieties of dinuclear, trinuclear and oligonuclear molecules, radicals and ions, including metal complexes having geometries such as tetrahedral (Td), square planar (D_{4h}), octahedral (O_h), etc; Walsh diagram; Evidence of MO pictures from spectra and reactivity; Explanation of spectrochemical and Nephelauxetic series; Molecular term symbols. **[12 lecture hours]**

Unit-2: Coordination Chemistry-II

Experimental evidence of metal-ligand overlap, spin orbit coupling constant and inter electronic coupling parameters in complex ion terms-vs-free ion terms, adjusted CFT, interpretation of general features of the electronic absorption spectra, vibronic coupling, intensity stealing, band broadening, effect of substitution, electronic structure and bonding of octahedral, tetrahedral complexes on the basis of simple symmetry and overlap principles, the MO energy level diagrams (with appropriate symmetry designation) of these complexes. **[12 lecture hours]**

Unit-3: Bioinorganic chemistry-2

Molybdenum containing enzymes: Nitrate reductase, Xanthine oxidase, Sulphate oxidase, cytochromes. Metal ions transport and storage proteins: ferritin, transferin, ceruloplasmin. Respiratory electron transport chain, cytochrome c oxidase, photosynthetic electron transport chain chlorophyll, PSI and PS-II, biological nitrogen fixation (nitrogenase). **[12 lecture hours]**

Unit-4: Chemistry of d-block elements:

Electronic configuration, oxidation state, redox and coordination chemistry, spectral and magnetic properties in different oxidation states, horizontal and vertical trends in respect of 3d, 4d and 5d elements (Ti-Zr-Hf, V- Nb-Ta, Cr-Mo-W, Mn-Tc-Re, Fe-Ru-Os, Co-Rh-Ir, Ni-Pd-Pt, Cu-Ag-Au and Zn-Cd- Hg). Dinitrogen and dioxygen complexes: synthesis, structure, bonding and reactivity. Uncommon oxidation states of transition metals - Fe(IV), Co(IV), Ni(III), Ru(IV), Os(IV), Pd(III /IV), Pt(III), syntheses and structures. **[12 lecture hours]**

Unit-5: Symmetry

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, identification of point groups, Symmetry of C60 fullerenes, Crystallographic symmetry, Hermann-Mauguin notation, optical activity and dipole moment. 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. Character table construction, Mulliken symbols. **[12 lecture hours]**

Topic name: Physical Chemistry (Theory)
Course Code: PG-CHE-CC-202
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Valency

Approximations in Quantum Chemistry. Born-Oppenheimer (B.O.) approximation. Avoided crossings and beyond B.O. approximation. Virial theorem and chemical bonding. Theories of valence: VB and MO. π-electron Hamiltonians: Hierarchy of assumptions. **[12 lecture hours]**

Unit-2: H-atom Problem

Cartesian and polar coordinates. Center of mass and relative coordinates. General forms of solutions and orbital specifications. Spherical harmonics. Real and complex orbitals. Role of constant motion.

[12 lecture hours]

Unit-3: Group Theory 1

Reducible and irreducible representations, Classes and Characters, Great Orthogonality theorem and related theorem, Projection operators, Direct product representation, Construction of SALC, Selection rules in spectroscopy, Study of normal modes, IR and Raman activity. **[14 lecture hours]**

Unit-4: Statistical Thermodynamics

Entropy and probability. MB distribution. Partition functions. Relevance to thermodynamics. PF for atoms and diatomics. Application to chemical/ionization equilibrium, Equipartition principle. Gibbs paradox and quantum statistics. Blackbody radiation. **[12 lecture hours]**

Unit-5: Biophysical Chemistry-1

Configuration and conformation of biological macromolecules. Membrane structure. Spectroscopic methods: UV-Vis and CD. Separation techniques: Gel Electrophoresis. Macromolecule-ligand binding and cooperativity. **[10 lecture hours]**

Topic name: Organic Chemistry (Theory)
Course Code: PG-CHE-CC-203
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Oxidising and reducing agents in organic synthesis

Oxidation: metal-based oxidants (Cr, Mn, Os, Ag, Ru and Pb); non metal-based oxidation: Swern oxidation, Moffat oxidation, hypervalent iodine based oxidants, CAN as oxidant.

Reduction: metal hydrides (B-H, Al-H, Zn-H, Sn-H, Si-H based reagents); hydrogenation; dissolving metal reductions; samarium iodide. **[12 lecture hours]**

Unit-2: Synthetic Methodology 1

Organoboron: Chemistry of organoboron compounds, carboranes, hydroboration, reactions of organoboranes (oxidation, protonolysis, halogenolysis, amination, isomerisation, carbonylation, cyanidation etc.), organoborane route to unsaturated hydrocarbons, allyl boranes, boron enolates.

Organosulphur: Sulphur stabilised anions and cations, sulphonium salts, chemistry of sulphur ylids.

[12 lecture hours]

Unit-3: Synthetic Methodology 2

Organophosphorus: Phosphorus ylides, Wittig reaction and its modifications. Phosphines and phosphites. Arbutsov reaction.

Organosilicon: Generalisations in silicon chemistry, Use of arylsilanes, vinylsilanes, epoxysilanes, allylsilanes. **[12 lecture hours]**

Unit-4: Photochemistry

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, cis-trans isomeriation, Paterno-Buchi reaction, Norrish type I and II reactions, photoreduction of ketones, di-pi-methane, oxo di-pi methane and aza di-pi methane rearrangements, Barton reaction, Hofmann-Loefflar-Freytag reactions, photochemistry of arenes, SRN1 reaction, photooxidation, Photoreaction in solid state. Method of generation and detection of radicals (ESR), radical initiators, reactivity pattern of radicals, substitution and addition reactions involving radicals, synthetic applications: cyclisation of radicals including various ring expansion, ring contraction, remote functionalisation and radical fragmentation reaction.

[15 lecture hours]

Unit-5: Natural Products II

Alkaloids: Definition and classification, general methods of isolation and structure elucidation, structure and synthesis of ephedrine, piperine, nicotine and papaverine. Biosynthesis of ephedrine and nicotine.

[9 lecture hours]

Topic name: Inorganic & Physical Chemistry (Practical)
Course Code: PG-CHE-CC-204(P)
(50 marks)
120 Practical hours 4 Credits

Inorganic Chemistry

A. Analysis of Alloys and Ores/Minerals

1. Quantitative estimation of Zn(II) and Cu(II) in brass sample by Volumetry and gravimetry
2. Quantitative estimation of iron in cast iron and steel.
3. Quantitative estimation of manganese in pyrolusite
4. Quantitative estimation of $CaCO_3$ in dolomite

B. Physical Chemistry 2

Experiments (Kinetics, equilibrium, electrochemistry, spectroscopy)

Topic name: Organic Chemistry (Practical)
Course Code: PG-CHE-CC-205(P)
(50 marks)
120 Practical hours 4 Credits

A. Preparation of selected organic compounds involving electrophilic substitution, addition, elimination and condensation reactions.
B. Separation and identification of solid organic compounds from their binary mixture.

SEMESTER-III

Topic name: Inorganic Chemistry (Theory)
Course Code: PG-CHE-CC-301
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Chemistry of elements

Metal –metal single and multiple bonding (pictorial MO approach). Bonding in dirhenium compounds Electronic transition and magneto properties. Isolobal and isoelectronic relationship. Synthesis, properties, reactions, structure and bonding of molybdenum blues, tungsten blue, ruthenium blue, tungsten bronze, ruthenium red, crutz-taube complex and vaskas compound. **[12 lecture hours]**

Unit-2: Application of organometallic Chemistry

Unique reactions in organometallic chemistry and catalysis: Coordinative unsaturation, Substitution, Oxidative addition, Insertion (migration), Isomerization, Reductive elimination; Catalytic converters; Alkene hydrogenation, Water gas shift reaction, Fischer Tropsch process. Hydroformylation (Oxo process), Carbonylation of olefins, Monsanto's acetic acid synthesis, Wacker oxidation (Pd-catalysed), Polymerization of olefins, Ziegler-Natta catalyst. **[12 lecture hours]**

Unit-3: Magnetochemistry

Magnetic properties of free ions (both first order and second order Zeeman effect to be considered), effect of spin orbit coupling on Sm^{+3} and Eu^{+3}.Antiferromagnetic interactions in inorganic compounds: Mechanism like – direct interaction, superexchange interactions and elucidation with poly nuclear metal complexes as well as oxide and halide salts of transition metals. Magnetic materials, super paramagnetism, magnetic behaviour of lanthanides and actinides. **[12 lecture hours]**

Unit-4: Chemistry of f-block elements

Lanthanides. Actinides and Super heavy elements. Electronic structure, differences between 4f and 5f orbitals. Stable oxidation states. Lanthanide and Actinide contruction, separation and isolation. Absorption spectra and magnetic properties. Comparative chemistry of d and f block elements, Comparative chemistry of Lanthanides and Actinides. Aqueous chemistry, coordination chemistry. Trans actinide elements, nuclear instability and synthesis chemistry of U and Pu. Periodicity of trans Lawrencium elements, super actinides. **[12 lecture hours]**

Unit-5: Analytical chemistry-II

Cyclic voltametry and coulometry: Basic principle, three electrode configuration. Solvents and supporting electrolytes. Representation of cyclic voltammogram, half wave potential, irreversible, reversible and quasi-reversible redox processes. Electron transfer at a constant potential, no. of electron transfer. Application in coordination chemistry (characterization, determination of redox potential), e.g. ferrocene, Co(II)/Co(III); Ni(II)/Ni(III); Cu(I)/Cu(II); $Ru(II)(bpy)_3$. Spectrochemical analyses. **[12 lecture hours]**

Topic name: Physical Chemistry (Theory)
Course Code: PG-CHE-CC-302
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Mathematical concepts

Basic mathematics, Elements of calculus, Extremum principles, constrained extremization, Power series: Convergence and divergence, Taylor series and Fourier series. Vectors and linear vector space: matrices. Applications. **[8 lecture hours]**

Unit-2: Quantum Chemistry

Variation method: Basis and applicability. Linear variation method-secular determinant. Many-electron systems: Closed and open shells, Antisymmetric principle and antisymmetrizer operator. Independent particle model (IPM). Self-consistent fields: Hartee and Hartee-Fock(HF) Theories. HF methods for closed shells. Implementation of HF method for closed shells: Roothan equation. HF theory and Koopmans' theorem. Problems with open-shell systems. Restricted and unrestricted HF methods (elementary idea). Electron correlation. Multideterminantal wave function and CI. Brillouin's theorem. Non-variational non-perturbative approximate methods-elementary exposure. Rudiments of Density Functional Theory: Expectation Value calculation using density: Kohn-Hohnenberg Theorems; Kohn-Sham equation for the ground state of many body systems; Fermi and Coulomb holes; exchange correlation functional. **[16 lecture hours]**

Unit-3: Theoretical Spectroscopy

Selection rule for vibrational spectra, anharmonic correction by perturbation - appearance of overtones, selection rule for rotational spectra, nuclear spin and energy levels, Stark effect, Raman scattering, selection rule for rotation-vibrational Raman effect. Nonlinear scattering- hyper –Raman, Stimulated and Resonance Raman spectra.

[12 lecture hours]

Unit-4: Statistical Mechanics -2

Phase space, ergodic hypothesis, Liouville's theorem, Concepts of different ensembles with applications to selective systems. Fluctuations. Prefect gas and the Sackur-Tetrode equation, System of interacting molecules, treatment of imperfect gases. Formulation of Quantum statistical mechanics: pure and mixed states, density matrix, quantum Liouville theorem and its consequences, Quantum statistics and ensembles. The specific heat of electron gas, Debye theory, Bose condensation. **[12 lecture hours]**

Unit-5: Group Theory -2

MO theory with applications to σ and σ* bonding and construction of hybrid orbitals. LFT with applications to splitting of terms and levels in different coordination environments and construction of energy level diagrams, Applications of symmetry principles in Woodward-Hoffman type reactions like dimerization of ethylene and Diels-Alder reaction. [**12 lecture hours]**

Topic name: Organic Chemistry (Theory)
Course Code: PG-CHE-CC-303
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: NMR Spectroscopy 2

Advanced Techniques and Applications of NMR Spectroscopy: ^{1}HNMR principles, Techniques for simplification of ^{1}H NMR spectra (Chemical techniques: deuteration, trifluoroacetylation, lanthanide shift reagents, chiral resolving agents; Instrumental techniques: use of higher magnetic field, spin decoupling, NOE); ^{13}C NMR principles, rules for carbon 13 calculations, relaxation processes, population transfer, selective polarization transfer, NMR shift reagents and their applications, basic two-dimensional sequence.
Two-dimensional (2D) NMR Spectroscopy: Application of ^{1}H and ^{13}C with advanced techniques (DEPT, COSY, NOESY, HETCOR) in structure elucidation of organic compounds. **[16 lecture hours]**

Unit 2: Mass Spectrometry

Theory and instrumentations. General rules for fragmentation. Basic fragmentation types of simple organic molecules having different functional groups. Different ionization techniques such as HR, CI, FAB and MALDI-TOF techniques. **[8 lecture hours]**

Unit-3: Stereochemistry 2

Stereochemistry of cyclic compounds: Conformations of monocyclic systems (small and medium ring compounds), 6-6, 6-5, 6-4, 5-5 bicyclic systems, 6-6-6, 6-5-6, 5-6-5, 5-5-5 tricyclic systems.
Dynamic Stereochemistry: Stereoselective reactions, enantioselective and diastereoselective reactions. Addition to carbon-carbon and carbon-hetero double bonds, epoxidation, dihyroxylation, amino-hydroxylation, hydrolysis, esterification etc. **[12 lecture hours]**

Unit-4: Asymmetric Synthesis

Enantio- and diastereoselective synthesis. Reactions of enolates (α–substitution), Addition to C=C double bonds (electrophile induced cyclization, iodolactonisation), Asymmetric hydroboration, Conjugate additions. Reduction of C=C double bonds, Aldol Reaction. Diels Alder Cycloaddition, Cyclopropanation, Oxidation, Epoxidation, dihydroxylation and aminohydroxylation. **[12 lecture hours]**

Unit-5: Organometallic Chemistry of Transitional Elements

Application of organotransition metals in organic synthesis, structural and mechanistic aspects. Davies rule, catalytic nucleophilic addition and substitution reaction, Coupling reaction-Heck, Stille, Suzuki coupling, Ziegler Naata reaction, Olefin metathesis, Tebbe's reagent, functional organometallic compounds. Pauson-Khand reaction, Volhsrdt co-trimerisation. Application of non-transition metals like Indium, tin, zinc. **[12 lecture hours]**

Topic name: Inorganic Special (Practical)
Course Code: PG-CHE-DSE-304(P) [A]
(50 marks)
120 Practical hours 4 Credits

1. Inorganic qualitative analysis (Less common elements).
2. Preparation of inorganic and coordination compounds and their characterization.
3. Chromatographic separation of ligands and metal complexes.

Topic name: Physical Special (Practical)
Course Code: PG-CHE-DSE-304(P) [B]
(50 marks)
120 Practical hours 4 Credits

Experiments (Kinetics, equilibrium, electrochemistry, spectroscopy, computer).

Topic name: Organic Special (Practical)
Course Code: PG-CHE-DSE-304(P) [C]
(50 marks)
120 Practical hours 4 Credits

1. Multistep Organic synthesis.
2. Column chromatographic separation of organic mixture.

Topic name: Generic Elective (Theory)
Course Code: PG-CHE-GE-313
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Air and Water pollution by chemical means

Air pollution: Primary pollutants and their origins, harmful effect of CO, NOx, SOx, hydrocarbon and other organic, photophysical smog, CFC'S, ozone hole, greenhouse effect, global warming, particulate matters, acid rain radioactive pollutants and their effects.

Water pollution: Aquatic pollutants, chemical, radioactive and thermal pollutants, basic gaseous and coloured inorganic and organic pollutants, pollutants in industrial effluents and sewage, Fertilizer waste, agricultural runoff, pesticides and other pollutants in the soil. As-pollution, F^-, NO_3^-/ NO_2^-, PO_4^{3-} pollutions. **[15 lecture hours]**

Unit-2: Treatment of water

Water treatment, municipal and industrial water, drinking water from sea. Removal of hardness. Chemical and electrochemical methods, ion exchange, reverse osmosis. **[5 lecture hours]**

Unit-3: Polymers

Introduction, types of polymers, classification of solvents; degree, extent and kinetics of polymerization; number and weight average molecular weights and their relation, determination of molecular weights by osmometry and viscometry, Advanced synthetic techniques for controlling molecular weight dispersity in synthetic polymers-Living polymerization (living ionic, living radical and living ring-opening polymerizations); block copolymers-synthesis, microstructure, and applications; Conjugated polymers and their electrical and opto-electronic properties.

[20 lecture hours]

Unit 4: Pesticides

Common pesticides: structures, production, applications and residual toxicity of gammaxane, aldrin, parathion, malathion, DDT, paraquat, decamethrin. **[10 lecture hours]**

Unit 5: Drugs

Concept and necessity of drugs and pharmaceuticals; synthesis and uses: aspirin, paracetamol, sulphadiazine, quinine, chloroquine, phenobarbital, metronidazole. **[10 lecture hours]**

SEMESTER-IV

Topic name: Inorganic Chemistry (Theory)
Course Code: PG-CHE-DSE-401(A)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Reaction mechanism of transition metal complexes

Energy profile of reactions, discussion on general reactivity of metal complexes, inert and labile complexes, different types of mechanisms (‘D’, ‘A’, ‘Ia’ and ‘Id’). Techniques for experimental measurements of reaction rates, techniques for fast reaction. Substitution reactions: Application of CFT, mechanism of ligand substitution in octahedral complexes, mechanism of isomerisation and racemisation, substitution reactions in square planar complexes. *Cis*- and *trans*- effects. **[12 lecture hours]**

Unit-2: Electron transfer reactions and twist mechanism

Mechanism of redox reactions with reference to metal complexes. Electron transfer reactions– outer sphere and inner sphere, atom transfer, induced electron transfer reactions, two electron transfer reactions, non complementary reactions, synthetic implications of electron transfer reactions, solid state electron transfer reactions. Electroprotic reactions. Twist mechanism of racemisation, inversion of configuration and associated process. **[12 lecture hours]**

Unit-3: Metal carbonyls, clusters, rings and cages

Metal carbonyls: Synthesis, structure and reactivity. Low nuclearity (M_3-M_4) and high nuclearity (M5-M10) carbonyl clusters. Metal-metal bonding (MO), skeletal electron counting, Isolobal analogue. Halide clusters of Nb, Ta, Mo, W, Re. Synthesis, structure and bonding. Interstitial Clusters-hydrides, carbides and nitrides. Metal-metal multiple bond: synthesis, structures and bonding(MO) and electronic transition.

[12 lecture hours]

Unit-4: Crystallography

Crystalline solid: single crystal and polycrystal (twinning problem) lattice, unit cell- primitive and nonprimitive unit cells, unit cell parameters and crystal systems. Crystal symmetry: point group elements and space group elements; 32 crystal classes, Hermann–Mauguin (HM) notations, distribution in different systems and stereographic projections. Space group-HM notations, space group in triclinic and monoclinic system. Indexing of lattice planes, Miller indices. Bragg's equation, reciprocal lattice and its relation to direct lattice; Bragg's reflection in terms of reciprocal latticesphere of reflection and limiting sphere; relation between dhkl and lattice parameters. **[12 lecture hours]**

Unit-5: Solid state chemistry

Defects in solids, line and plane defects. Deterination of equilibrium concentration of Schottky and Frenkel defects, Stoichimetric imbalance in crystals and non- stoichiometric phases, Color centres in ionic crystals. Band theory, band gap, metals, insulators, semiconductors (intrinsic and extrinsic), dopping, rectifiers and transistors. Bonding in metal crystals: Free electron theory, electronic specific heat, Hall effect, electrical and thermal conductivity of metals, Superconductivity, Meissner effect, basic concepts of BCS (Bardeen-Copper-Schriffer) theory. **[12 lecture hours]**

Topic name: Physical Chemistry (Theory)
Course Code: PG-CHE-DSE-401(B)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Solids

Reciprocal lattice, Structure factor, Fourier synthesis, Band theory, band gap, metals and semiconductors – intrinsic and extrinsic semiconductors, superconductors. **[8 lecture hours]**

Unit-2: Electric and Magnetic Properties of Matter

Dielectric polarization; Debye equation and its limitation; Onsager's reaction field model; electric polarizability of molecules; magnetic susceptibility - diamagnetic and paramagnetic, Courie law, Molecular interactions Hamiltonian in absence and presence of external fields, forces in molecules, Hellmann-Feynmann theorem, perturbative treatment of electric polarisability, intermolecular interaction - calculation of dispersion energy, the London formula

[12 lecture hours]

Unit-3: Non-ideal Systems

Virial equations, second Virial coefficient; determination of intermolecular potentials employing hard-sphere, square-well and hybrid potential models; non-ideal solutions; partial molar quantities and their determinations, Duhem-Margules equation and its applications, regular solutions and excess thermodynamic functions. **[12 lecture hours]**

Unit-4: Thermodynamics of Irreversible Processes

Limitations of classical (equilibrium) thermodynamics, entropy production in some simple irreversible processes, the concept of forces and fluxes, linear phenomenological relations; Onsager reciprocity relation -derivation from fluctuation theory; Curie-Prigogine principle - statement and proof using one scaler and one vector force, illustrations; Saxen's relations in connection with electrokinetic phenomena and their proof using Onsager reciprocity relations, stationary states: variation of entropy production with time, Prigogine's criterion for establishment of stationary state, applicability of Le Chateliar's principle on stationary states. **[16 lecture hours]**

Unit-5: Electrochemistry

Introduction, ion-solvent interaction: Born model and Born equation, enthalpy of ion-solvent interaction and its calculation, Eley-Evan model, solvation number and methods for determination of solvation number, ion association: Bjerrum equation, fraction of ions associated, ion association constant.

[12 lecture hours]

Topic name: Organic Chemistry (Theory)
Course Code: PG-CHE-DSE-401(C)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit 1: Alkaloids

Structural types, general introduction to phenylethylamine, pyrrolidine, pyridine, indole, isoquinoline type alkaloids. Quinine, morphine, yohimbine, reserpine, strychnine, lysergic acid and their uses.

[12 lecture hours]

Unit 2: Steroids

Chemistry of cholesterol, bile acids and some important steroidal hormones. Structure and biosynthesis of cholesterol and other related steroids. **[8 lecture hours]**

Unit 3: Carbohydrate Chemistry

Conformational analysis of monosaccharides (pentoses and hexoses). Structure of maltose and gentiobiose. Protection and deprotection. *O*-glycosylation, C-glycosylation, Deoxysugars, amino sugars, glycal sugars and their synthetic aspects. Carbohydrates as chiral pools in organic synthesis. **[12 lecture hours]**

Unit 4: Bioorganic Chemistry of Amino Acids

Introduction – importance of amino acids and peptides in chemical biology; Amino acids and their asymmetric synthesis; Amino acids as building blocks; Chemistry of peptide bonds; synthesis of peptides, N-protection, Carboxy protection, activating agents, determination of N-terminus and C-terminus, Edman

degradation; Peptide secondary structures and tools for stabilization; Synthetic peptides of importance, solid phase synthesis of peptides. **[16 lecture hours]**

Unit 5: Synthesis of Advanced Materials

Synthesis of novel advanced materials by new generation catalysts via ROMP (ring opening metathesis polymerization) reactions, nano structure material catalysis reaction, applications of nano-gold, nano-palladium, nano-copper in organic synthesis, carbon nanotubes (synthesis, forms, properties, applications). **[12 lecture hours]**

Topic name: Inorganic Chemistry (Theory)
Course Code: PG-CHE-DSE-402(A)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Inorganic Special - 402[I]

Unit-1: Mössbauer spectroscopy

Principle, experiment, line width, centre shift, quadrupole interaction, magnetic interaction, information on spin and oxidation states, structure and bonding, spin transition from spectra of different Mössbauer active nuclei in various environments. Application of Mössbauer spectroscopy for inorganic compounds. **[12 lecture hours]**

Unit-2: EPR spectroscopy

Principle, spin Hamiltonian (comparison to NMR spectra), energy of spinning electron in a magnetic field, EPR-instrumentation, representation of EPR spectrum, X-band and Q-band spectra, line width, hyperfine splitting, magnetically equivalent and non-equivalent sets of nuclei, g-anisotropy, spectra of simple organic free radicals: expected number of lines, intensities. Spectra of transition metal complexes, metal hyperfine anisotropic spectra, zero field splitting, application: determination of oxidation state of metal ion in samples. **[12 lecture hours]**

Unit-3: NMR spectroscopy

Principle of NMR spectroscopy, ^{1}H NMR spectra of paramagnetic coordination compounds, dipolar and contact shifts, magnetic susceptibility and resonance shifts. ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{31}P, ^{51}V –NMR spectra. Identification of compounds like H_3PO_3, H_3PO_2, HPF_2, P_4S_3. Exchange reaction- exchange in water, factors effecting line width, evaluation of thermaodynamic parameters with NMR, determination of reaction order, rate constant etc. from NMR. NMR spectra of paramagnetic ions. Contact shifts. Factors contributing the magnitude of chemical shift. Applications involving the magnitude of coupling constant-J, ^{13}C-H, JPt-P, JP-F etc. **[12 lecture hours]**

Unit-4: IR, Raman,

Basic principle and applications of IR spectroscopy for inorganic compounds. Raman spectroscopy: theory, instrumentation, mechanism of Raman effect, effect in solid, liquid and gases, use of symmetry consideration to determine the number of active infrared and Raman lines, differences between IR and Raman spectra. **[12 lecture hours]**

Unit-5: UV-visible spectroscopy, CD and ORD spectroscopy

Electronic Spectroscopy, Basic principles, electronic trasition in organic, inorganic and organometallic molecules and applications. CD and ORD spectroscopy: basic principle, symmetry origin of the optical activity of molecules, the phenomenon of optical rotator dispersion (ORD) and circular dichrosim (CD), the Cotton effect, application. **[12 lecture hours]**

Topic name: Physical Chemistry (Theory)
Course Code: PG-CHE-DSE-402(B)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Polymer Chemistry -2

Molecular weights and molecular weight distributions and their determinations (viscometry, osmometry, light scattering, size-exclusion chromatography; Principles of macromolecular synthesis: step-growth vs. chain-growth polymerizations.Advanced synthetic techniques for controlling molecular weight dispersity in synthetic polymers-Living polymerization (living ionic, living radical and living ring-opening polymerizations); block copolymers-synthesis, microstructure, and applications; Conjugated polymers and their electrical and opto-electronic properties. Structure & properties of polymers – morphology & order in crystalline polymers, polymer chains, effect of strain, crystallization & melting; structure & physical properties, melting point, effect of chain flexibility & other steric factors, entropy & heat of fusion; glass transition temperature; relation between Tm & Tg, effect of molecular weight, chemical structure, chain topology, branching & crosslinking, property requirements & polymer utilization. **[18 lecture hours]**

Unit-2: Biophysical Chemistry-2

Introduction to the structural hierarchy in proteins, nucleic acids and lipids, basic features of primary, secondary, tertiary and quaternary structures of proteins, nucleic acid and lipids, explanation of various interactions determining the structures of biomolecules features and importance of hydrogen bonding in biomolecules and hydrophobic effect in biological structures. Protein conformational transition, helix coil transition, protein folding, common folds in proteins, Ramachandran plot, supercoiled 42 structure of nucleic acid, organized structure of amphiphile aggregates. **[15 lecture hours]**

Unit-3: Corrosion

Corrosion and it's control: Introduction, Electrochemical theory of corrosion, Factors affecting the rate of corrosion: ratio of anodic to cathodic areas, nature of corrosion product, nature of medium – pH, conductivity and temperature. Types of corrosion - Differential metal and differential aeration (pitting and water line). Corrosion control: Anodizing – Anodizing of aluminum, Cathodic protection - sacrificial anode and impressed current methods, Metal coatings – Galvanization. Corrosion Penetration Rate (CPR), numerical problems on CPR. **[9 lecture hours]**

Unit-4: Kinetics-2

Rate processes and some physical phenomena. Statistical approach to rate theory: Hinshelwood, RRK and RRKM theories. **[6 lecture hours]**

Unit 5: Computational Chemistry

Introduction to computational chemistry and molecular modeling, potential energy surface, energy minimization, introduction to computational quantum mechanics and classical force field models, basic computations with reference to simple chemical and biological molecules. **[12 lecture hours]**

Topic name: Organic Chemistry (Theory)
Course Code: PG-CHE-DSE-402(C)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Heterocyclic Chemistry I

Synthesis and reactivity of quinoline, isoquinoline, pyrazole, imidazole, oxazole, thiazole, isooxazole, isothiazole and their applications in organic synthesis. **[14 lecture hours]**

Unit 2: Supramolecular Chemistry

Basic concepts of supramolecular chemistry, different non-covalent forces (e.g. H-bonding, cation-π, anion-π, π-stacking, hydrophobic, hydrophilic interactions etc.) leading to strong bonding of guest molecules to the hosts, thermodynamics of host-guest complexation, solvent effects and salt effects in complexation, design principle of host molecules. New molecular receptors, Crown ether, Sidero force, Cyclophanes, Cyclodextrin and their application in specific recognition processes., Supramolecular reactivity and catalysis, Switching devices, self-assembly, supramolecular gels, self-replication, supramolecular transportation. **[14 lecture hours]**

Unit-3: Medicinal Chemistry 1

Antibiotics – Penicillins, Cephalosporins, tetracyclins, newer generation of antibiotics. Vitamins - Definition of vitamins and coenzymes, classification of vitamins, mechanism of function with synthesis of vitamin A, B1, B6 and folic acid, etc. Drugs - Introduction and classification of drugs, brief discussion on drug targets. Sulphur drugs, anti tubercular drugs, anti diabetic drugs and newer generation of antacids.

[12 lecture hours]

Unit 4: Green Chemistry

Green Chemistry: Introduction, principles, green synthetic methods, catalytic methods, organic synthesis in aqueous media, ionic liquid, supercritical fluids, MCR reactions, microwave-induced organic reactions, real-world cases of green chemistry.

[10 lecture hours]

Unit-5: Bio-active Molecules

Chemistry of porphyrins, lipids, polyunsaturated fatty acids, arachidonic acid cascade, prostaglandins – structure and synthesis. Steroids: General methods of study and structural type. Chemistry of cholesterol, hormones, bile acids, vitamins of D-group, diosgenin.

[10 lecture hours]

Topic name: Inorganic Chemistry (Theory)
Course Code: PG-CHE-DSE-403 (A)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Chemical applications of group theory

Splitting of orbitals and free ion terms in weak crystal fields, symmetries and multiplicities of energy levels in strong crystal fields, correlation diagram, Vanishing of quantum mechanical integral, transition probability, selection rules. Justification of Laporte selection rule. Symmetry of hybrid orbitals. Determine the symmetry and combinations of Ligand group Orbitals (LGO) and metal orbitals in octahedral, square planar, tetrahedral and other ligand environments using of projection operator. Construction of qualitative MO energy level and interaction diagram on the basis of symmetry considerations only. Drawing of LGO and MO diagrams. **[12 lecture hours]**

Unit-2: Organometallic Chemistry –II

Chemistry of transition metal complexes with cyclic polyenes: 3-6 membered ring systems. Sandwitch and non sandwitch complexes. Organometallic chemistry of heterocyclc ligands (N,B,O). Multidecker sandwitch complexes. Bioorganometallic chemistry, Organometallic polymers. **[12 lecture hours]**

Unit-3: Inorganic photochemistry

Introduction to inorganic photochemistry, photophysical and photochemical process, characteristics of the electronically excited states of inorganic compounds, ligand field states, charge transfer states, Frank Condon (FC) states, THEXI and DOSENCO states, kinetics of photochemical process, photosensitization. Transition probabilities, Transition moment integral and its applications. Selections rules. Jablonski diagram, Fluorescence and phosphorescence, delayed fluorescence, quantum yield, mechanism and decay kinetics of photophysical processes. Fluorescence quenching (dynamic and static), Stern-Volmer equation. Photochromism; chemical actinometry, photochemical reaction of coordination compounds.

[12 lecture hours]

Unit-4: Non transition metal chemistry:

Silicon halides, Phosphorous halides, acids, oxyacids of phosphorous, phosphazenes; Sulfur halides, oxo acids of sulphur; structural features and reactivity of N-S heterocycles. Inorganic Polymers: $(BN)_X$, Borates, $(SN)_X$, $(PS)_X$, PNX_2, Silanes, Silicates, Silocones, Silanols. **[12 lecture hours]**

Unit-5: Supramolecular chemistry and, molecular materials:

Origin of supramolecular chemistry-"Chemistry beyond the molecules". Concepts and terminology of supramolecular chemistry. Natural types of supramolecular interactions (Hydrogen bonding, van der Waal"s interaction, π-stacking, CH---π interaction. Supramolecular chemistry in inorganic perspective. Inorganic crystal engineering and design principle of metal organic framework (MOF) and inorganic-organic hybrid material. Application of MOFs in material science. **[12 lecture hours]**

Topic name: Physical Chemistry (Theory)
Course Code: PG-CHE-DSE-403 (B)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1: Perturbation Theory

Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications. Brillouin-Wigner theory. Matrix perturbation. Degenerate perturbation theory-Stark effect. First and second order lifting of degeneracy. **[8 lecture hours]**

Unit-2: Quantum Mechanics-2

Stern-Gerlach expt., Hilbert space, Dirac notation, generalized uncertainty principle, position and momentum space rep. Continuous vs discrete basis, Delta function and Fourier transformation, Pictures-Schrodinger-Heisenberg-Dirac.Time ordering, Dyson series up to second order correction, Fermi-Golden rule, Einstein A, B coefficient, Rabi oscillation, Sudden approximation. Gell-Mann and Low theorem. Symmetry in quantum mechanics, Parity and time reversal. Harmonic oscillator (wavefunction and operator methods), Coherent state, Constants of motion. Representations. Commutation relations. Step up/down operators. Quantization. Spin and Pauli matrics. Matrix representations of total angular momentum operators. Many electron systems. **[18 lecture hours]**

Unit-3: Principle of Lasers and its applications

Two level transition (absorption, induced and stimulated emission), Einstein model for two levels transition, Principle of Maser and Laser action. Population inversion (two/three/four level systems), Basic element in laser (resonator, Gain medium, Pumping technique), Characteristics of laser radiation (coherence: temporal/spatial; polarization, monochromaticity, intensity), Single mode laser (solid/ gas laser: Ruby, Nd:YAG, Ar-ion, CO_2, Excimer etc.) tunable laser (Dye laser), Harmonic generation, Application of laser (chemical problem, medicinal and industrial). **[16 lecture hours]**

Unit-4: Photochemistry

Production of excited states, singlet and triplet states, radiative and non-radiative processes, fluorescence and phosphorescence: mirror image relationship, quantum yield and life-time; phenomenological approach of quenching, transient effects; properties of excited states: dipole moment, pKa, energy transfer, photoinduced electron transfer, excimers and exciplexes; special photochemical reactions, flash photolysis, laser flash photolysis. **[12 lecture hours]**

Unit-5: FT-NMR Spectroscopy

Introduction to pulsed-FT-NMR. Product-operator formalism of 1D and 2D NMR. Determination of three-dimensional structure of molecules using NMR spectroscopy. **[6 lecture hours]**

Topic name: Organic Chemistry (Theory)
Course Code: PG-CHE-DSE-403 (C)
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit 1: Total synthesis of natural products

Total synthesis of longifolene, reserpine, juvabione, aphidicolin and Fredericamycin A and Prostaglandins (PGE_2, $PGF_{2\alpha}$), taxol etc. **[12 lecture hours]**

Unit 2: Biogenesis and Biosynthesis of Natural Products

Biogenesis: Precursors, primary and secondary metabolites. Acetate hypothesis. Mevalonate and Shikimic acid pathways. General principles involved in the biosynthesis of amino acids, alkaloids, steroids and terpenoids. Biosynthesis of selected natural products: L-tryptophan, quinine, estrone, taxol.

[12 lecture hours]

Unit 3: Natural Oxygen Heterocycles

Naturally occurring oxygen heterocyclic compounds: Natural pigments, polyphenolics and other anti-oxidants. **[12 lecture hours]**

Unit 4: Medicinal Chemistry II

Chemical basis of disease states, definition and classification of drugs and theoretical aspects of drug action. Drug metabolism and drug excretion. Qualitative and quantitative structure activity relationship. Concepts of drug dosing and drug half-life, drug tolerance and physical dependence, drug potency and therapeutic index (LD-50 & CD-50). Mechanism of action of NSAIDs as pain killers and statin group of drugs to prevent atherosclerosis. Concept of prodrugs, pharmacophores and lead compounds. Molecular modification of drugs. Definition, classification and mechanism of action of antibiotics.

[12 lecture hours]

Unit 5: Advanced Heterocyclic Chemistry

Synthesis and reactions of aziridines, azitidines, imidazoles, oxazoles, thiazoles, isoxazoles, pyrazoles and their benzo derivatives. Pyrimidines, pyridazines, pyrazines, purines, pteridines. Nomenclature of bicyclic and tricyclic fused system heterocycles. Role of heterocyclic compounds in biological systems. Application of heterocycles in pharmaceutical and electronic industry. **[12 lecture hours]**

Topic name: Dissertation (Practical)
Course Code: PG-CHE-DSE-404(P) [A]
PG-CHE-DSE-404(P) [B]
PG-CHE-DSE-404(P) [C]
(50 marks=30+20)
120 Practical hours 4 Credits

Unit-1

Project Work

Research work / Review work to be decided in consultation with the concerned teacher. The work has to be carried out under the supervision of the in charge and a research report (Research work / Review work) has to be submitted.

Unit-2

Seminar Lecture has to be delivered on the total work carried out. It will involve power point presentation. Grand viva.

Topic name: Environmental Chemistry and Measurement (Theory)
Course Code: PG-CHE-SEC-405
(50 marks=40 End SEM Exam+10 Internal)
60 Lecture hours 4 Credits

Unit-1:

Chemical Toxicology: Trace elements and their chemical speciation with special reference to Cu, Zn, Cd, Hg, Pb, Ag, Sb,Se, Ti, Si, Be etc. Toxic chemical in air, water, soil, diet, fertilizer, their effects and remedial measures. Metal ion toxicity, metal dependent diseases, remedial measures, bio-mineralogy.

[10 lecture hours]

Unit-2: Pollution control measures

Removal of particulate matter, CO, SO_2, NOx, H_2S and organics from air, treatment of auto exhaust and few gases, electrostatic precipitator, absorption and adsorption and combustion techniques. Removal acidic, basic, inorganic and organic, coloured pollutants from water, chemical and microbial method. Treatment of Industrial effluents from paper, jute, textile, leather, cement, rubber plastic, fertilizer electroplating industry, thermal power plant, radioactive waste disposal. **[10 lecture hours]**

Unit 3: Advanced Spectroscopy

Basic principle, instrumentation and application of absorption and emission spectroscopy (atomic and molecular): Fundamental Laws of photometry, Limitation of absorption and emission measurement, Photometric titration, Fluorescence quenching (Static and Dynamic), Time resolved measurement, Qualitative and quantitative analysis. Jablonski diagram, various processes occurring subsequent to excitation – radiative and non-radiative transitions, fluorescence spectroscopy, fluorescence quenching,

Stern-Volmer plots, determination of fluorescence lifetime, single molecule spectroscopy, femtosecond spectroscopy. **[20 lecture hours]**

Unit 4: Food additives

Food flavour, food colour, food preservatives, artificial sweeteners, acidulants, alkalies, edible emulsifiers and edible foaming agents, sequestrants-uses and abuses of these substances in food beverages.

[10 lecture hours]

Unit 5: Fats and oils

Natural fat, edible and inedible oil of vegetable origin; common fatty acids; glycerides; hydrogenation of unsaturated oil, production of vanaspati and margarine. **[10 lecture hours]**

SUGGESTED BOOKS FOR INORGANIC CHEMISTRY

1. Advanced Inorganic Chemistry – F. A. Cotton & G. Wilkinson
2. Advanced Inorganic Chemistry, 6th Edn, John Wiley & Sons, Inc, New York, 1999 – F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann
3. Analytical Chemistry – G. D. Christian
4. Analytical Chemistry, Principles – J. H. Kennedy
5. An Introduction to Inorganic Chemistry – K. F. Puecell & J. C. Kotz
6. Bioinorganic Chemistry – R. W. Hay
7. Bioinorganic Chemistry, Books & Allied (P) Ltd. Kolkata 2007 – A. K. Das
8. Chemical Application of Group Theory – F.A. Cotton
9. Chemistry of The Elements – N. N. Greenwood & A. Earnshaw
10. Concept and Model in Inorganic Chemistry – Douglass, McDanniel & Alexander
11. Comprehensive Coordination Chemistry – G. Wilkinson, R. A. Gillard & J. A. McCleverty (eds)
12. Cluster Molecules of the p-Block Elements, Oxford University Press, Cambridge, 1994 – C. E. Housecroft
13. Coordination Chemistry – S. F. A. Kettle
14. Elements of Bioinorganic Chemistry – G. N. Mukherjee & A. Das
15. Fundamentals of Analytical Chemistry – D. A. Skoog, D. M. West and F. J. Holler
16. Inorganic Chemistry – J. E. Huheey, E. A. Keiter & R. L. Keiter
17. Introduction to Ligand Field Theory – C. J. Ballhausen
18. Introduction to Ligand Field – B. N. Figgis
19. Inorganic Chemistry – D. F. Shriver, P. W. Atkins & C. H. Langford
20. Inorganic Chemistry, Viva Books Pvt Ltd, New Delhi, 2001 – G. Wulfsberg
21. Inorganic Chemistry, 3rd Edn, Pearson Education Ltd, Essex, England, 2008 – C. E. Housecraft and A. G. Sharpe
22. Inorganic Chemistry – A. G. Sharpe
23. Introduction to Bioinorganic Chemistry – D.R. Williams
24. Molecular Electronic Structure of Transition Metal Complexes, McGraw-Hill, London, 1979 – C. J. Ballhausen
25. Symmetry Orbitals & Spectra – Jeffe & Archin
26. Symmetry in Chemistry – Jeffe & Archin
27. Symmetry in Molecules – J. M. Hollar

28. Theoretical Approach to Inorganic Chemistry – A. F. Williams
29. Theoretical Inorganic Chemistry – M. C. Dey and I. Selbin
30. Structural Inorganic Chemistry, 5Th Edn, Oxford University Press, Oxford, 1984 – A. F. Wells

Books for Practical

1. Quantitative Inorganic Analysis – G. Charlot & D. Bezier (translated by R. C. Murray)
2. Quantitative Chemical Analysis – I. M. Kolthoff, E. B. Sandel, J. Meehan and S. Bruckenstein
3. Advanced Experiments in Inorganic Chemistry – G. N. Mukherjee
4. Vogel's Textbook of Quantitative Chemical Analysis - G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney

SUGGESTED BOOKS FOR PHYSICAL CHEMISTRY

Books for Theory

1. Physical Chemistry: A Molecular Approach – D. A. McQuarrie, J. D. Simon
2. Physical Chemistry – R. S. Berry, S. A.Rice, J. Ross
3. Introduction to Atomic Spectra – H. E. White
4. Quantum Mechanics– J. L. Powell, B. Crasemann
5. Introduction to Quantum Mechanics– D. J. Griffiths
6. Introduction to Quantum Mechanics – L. Pauling, E. B.Wilson
7. Quantum Chemistry – I. N. Levine
8. Coulson's Valence– R. McWeeny
9. Chemical Application of Group Theory– F. A. Cotton
10. Group theory and chemistry–D. M. Bishop
11. Chemical Kinetics – K. J. Laidler
12. Foundations of Chemical Kinetics- S. W. Benson
13. Theoretical Chemistry- S. Glasstone
14. Fundamentals of Statistical and Thermal Physics – F. Reif
15. Statistical Mechanics – R. K. Pathria
16. The Principles of Chemical Equilibrium – K. Denbigh
17. Thermodynamics and Introduction to Thermostatics – H. B. Callen
18. Physics and Chemistry of Surfaces – N. K. Adams
19. Physical Chemistry of Surfaces – A.W. Adamson
20. Principles of Physical Biochemistry – K.V. van Holde, C. Johnson, P. S. Ho
21. Physical Chemistry of Macromolecules – C. Tanford
22. Polymer Chemistry – P. J. Flory
23. Essential of Physical Chemistry, S. Chand Publishing, India, 2010 – A. Bahl, B. S. Bahl, and G. D. Tuli
24. Atkin's Physical Chemistry: International Oxford University Press, 2018, 11th edition – P. W Atkins
25. Physical Chemistry, Cengage India Private Limited, 2017, 2nd edition – D. W. Ball
26. Functional Monomers and Polymers – K. Takemoto, R. M. Ottanbrite and M. Kamachi
27. Macromolecules: Structure and Function, Prentice Hall of India, 2001 – F. Wold
28. Physics and Chemistry of Polymers, Blackie Academic and Professional, 2014 – J. M. G. Cowie
29. Contemporary Polymer Chemistry, Prentice Hall, 2017 – H. R Alcock and F. W. Lamb
30. Textbook of Polymer Science, Wiley India Pvt. Ltd., 2014 – F. W. Billmeyer Jr.
31. Solid State Chemistry-An Introduction, 3rd Edition. CRC Press, 2005 – L. E. Smart, E. A. Moore
32. Modern Molecular Photochemistry, Univ. Science Books, 1991 – N. J. Turro
33. Statistical Mechanics, Viva Books Pvt. Ltd., New Delhi, 2003 – D. A. McQuarrie

34. Statistical Mechanics, 3rd Edition. Elsevier, 2016 – R. K. Pathria and Paul D. Beal
35. An Introduction to Statistical Thermodynamics, Dover Publication, 2018 – T. L. Hill
36. Statistical Mechanics for Chemistry and Material Science, CRC Press, 2018 – B. Bagchi
37. Physical Chemistry-A molecular approach, 1st Edition.Viva, 2010 – McQuarie and J. Simon

Books for Practical

1. Practical Physical Chemistry – A.M. James, F.F. Prichard
2. Findlay's Practical Physical Chemistry – B.P. Levitt
3. Experimental Physical Chemistry – Shoemaker and Ga
4. Experimental Physical Chemistry, Tata McGraw Hill, 1984 – R. C. Das and B. Behara
5. Advanced Practical Physical Chemistry, Goel Publishing House, 1991 – J. B. Yadav
6. Findley's Practical Physical Chemistry, 9thEdition. Longman Group Ltd., 1993 – B. P. Levitt
7. Practical Physical Chemistry, Lomgman, 1994 – A. M. James and F. E. Prichard
8. Experimental Physical Chemistry, 1st Edition. Oxford University Press, 1995 – G. P. Mathews
9. Physical Chemistry Practical, New Central book Agency, 2012 – K. Maity and N. K. Ghosh
10. Senior Practical Physical Chemistry, R. Chand & Co., New Delhi, 2014 – B. D. Khosla, V. C. Garg and Adarsh Gulati
11. Experiments in Physical Chemistry, McGraw Hill, 2015 – Shoemaker and Garland
12. Practical Physical Chemistry, M V Learning, 2017 – B. Viswanathan and P. S. Raghavan

SUGGESTED BOOKS FOR ORGANIC CHEMISTRY

Books for Theory

1. Advanced Organic Chemistry Part A & Part B, Springer 2007 – F. A. Carey and R. J. Sundburg
2. Organic Chemistry, Oxford University Press, 2012 J – Clayden, N. Geeves and S. Warren
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, John Wiley, 2005 – Jerry March
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PG- Coordinator
Department of Chemistry
Murshidabad University
Berhampore, W.B., 742101