



PG Prospectus 2024 Department of Chemistry Bidhannagar College Salt Lake, Kolkata- 700064

# **Brief History of the Department**

The Department of Chemistry at Bidhannagar College is one of the best centres for undergraduate and postgraduate teaching in Chemistry under the West Bengal State University. Chemistry has been taught here at the undergraduate honours level since 1985 under the affiliation of University of Calcutta. The college came under the affiliation of newly established West Bengal State University in 2008. The academic curriculum has been extended to postgraduate section (autonomous) in 2013. The overall performance of our students in the university examinations as well as in the national level competitive examinations is impressive.



# **Present Faculty strength**

Posts	Sanctioned	Filled
Professor	01	00
Associate Professor	14	02
Assistant professor	14	07

# Department of Chemistry, Bidhannagar College

# Faculty profile



Sl No	Name	Qualification	Designation	Specialization
1	Sanat Kumar Saha	Ph.D.	Associate Professor& Head	Physical Chemistry
2	Arup Kumar Adak	Ph.D.	Associate Professor	Inorganic Chemistry
3	Rajarshi Chatterjee	Ph.D.	Assistant Professor	Inorganic Chemistry
4	Anisur Rahaman Molla	Ph.D.	Assistant Professor	Organic Chemistry
5	Arabinda Mandal	Ph.D.	Assistant Professor	Inorganic Chemistry
6	Shubhankar Samanta	Ph.D.	Assistant Professor	OrganicChemistry
7	Susanta Kumar Manna	Ph.D.	Assistant Professor	OrganicChemistry
8	Tirtha Pada Majhi	Ph.D.	Assistant Professor	OrganicChemistry
9	Rituparna Biswas	Ph.D.	Assistant Professor	Inorganic Chemistry



# **Retired Guest Faculty**

Sl No	Name of the Teacher	Qualification	Institution Last served	Designation
1.	Dulal Chandra Mukherjee	Ph.D.	University of Calcutta	Former Professor
2.	Sanjib Bagchi	Ph.D.	University of Burdwan	Former Professor
3.	Samita Basu	Ph.D.	SINP Kolkata	Former Senior Professor
4.	Achintya Kumar Sarkar	Ph.D.	Bidhannagar College	Former Professor
5.	Gurucharan Mukhopadhyay	Ph.D.	Bidhannagar College	Former Associate Professor
6.	Nikhil Ranjan Pramanik	Ph.D.	Bidhannagar College	Former Associate Professor

# **Present staff**

Sl. No.	Name of Technical Staff	Designation	
1.	Biplab Sarkar	Laboratory Attendant	
2.	Subha Mondal	Laboratory Attendant	

# **Admission Procedure, Courses offered, No of seats**

**1. Admission Procedure:** Admission is centrally organized by the college as per West Bengal State University rules and notified in due time. Interested candidates must follow the college website (<u>https://www.bidhannagarcollege.org</u>) for regular update of the admission process.

#### 2. Courses offered:

#### a) B.Sc. Honours in Chemistry

#### b) M.Sc. in Chemistry

The post-graduate course shall comprise a total credit of 92 (ninety-two) distributed over the four semesters in two years. The courses shall be grouped as Departmental core courses, Department specific electives, Skill Enhancement Course (SEC), Generic Elective Course (GEC) and Ability Enhancement Comprehensive Course (AECC). Detailed syllabus of the course is given at the end (page 13-34).

#### 3. Intake capacity:

Course	No of seats
B.Sc. (Hons in Chemistry)	63
M.Sc. in Chemistry	38

# **Departmental Infrastructure**

The Department of Chemistry is spread over three wings of ground floor and includes the chamber of HOD, one staff room, four laboratories, one research laboratory, two compounding rooms, five dedicated lecture rooms including one smart class room, two store rooms and one instrument room for PG experiment. A well-stocked seminar library is also a part of the facilities available for the benefit of both UG & PG students and teachersmaintained by a faculty member.



**Smart Classroom** 



Laboratory

### Other Facilities available

- One sophisticated UV-Visible spectrophotometer
- Metler analytical balance (0.0001g)
- Rotary evaporator
- Computer with internet facility
- Low temperature bath
- Regular instruments/equipments as demanded by curriculum



**UV-Visible Spectrophotometer** 



**Rotary Evaporator** 



**Metler Analytical Balance** 

# **Research activity**

Active research work is carried out in the Department in a dedicated research laboratory assigned for the purpose and have regular publications in national/international journal of repute. Currently two major research projects are running in the Department.



**Research Laboratory** 

# **Extracurricular activities**

• The Department regularly organizes State/National level seminars in collaboration with other Institutes/bodies for enrichment of both students and faculty members.



• Wall magazines, posters are prepared by the present students on recent topics of Chemistry and displayed in dedicated spaces of the Department.



 Students are encouraged to participate in academic activities like seminars, other academic activities organized by different institutes e.g. Chemistry quizzes, laboratory visits etc. and their performances are praiseworthy.



Educational tour at IIT-KGP

# Academic achievements of PG students in recent past

Sl	Name of the	Achievement	Year	Current position
No	student			
1	Anusuya Saha	Project Fellow	2018	Research Fellow at CSIR Centre
				for Salt & Marine Chemical
				Research Institute
2	Manali Basu	Qualified UGC-NET	2018	Research Fellow at SINP Kolkata
3	Rajib Molla	Qualified CSIR-NET JRF	2018	Research Fellow at IISER Bhopal
		(Rank- 42)		
4	Anindya Sarkar	Qualified CSIR-NET JRF	2018	Research Fellow at IIT Kanpur
5	Sourav Dutta	Qualified CSIR-NET JRF	2019	Research Fellow at IACS Kolkata
6	Samim Sahaji	Qualified for Maulana	2019	Research Fellow at Bose Institute,
		Azad National		Kolkata
		Fellowship for Minority		
		Students		
7	Dipanwita Palit	Qualified CSIR-NET JRF	2020	Research Fellow at IISER Bhopal
8	Dibyendu Biswas	Qualified CSIR-UGC	2020	Research fellow at University of
		NET LS		Calcutta
9	Arka Biswas	Qualified GATE	2021	Research Fellow at Central Salt and
				Marine Chemical Research
10	Sumana	Qualified CSIR-NET JRF	2022	Research fellow at University of
	Mazumder	(Rank- 57)		Calcutta
11	Parag Mistry	Oualified CSIR-NET JRF	2022	Research Fellow at IIT Ropar
	6 5	(Rank- 121)		1
12	Somsubhra Kundu	Oualified CSIR-NET JRF	2022	Research Fellow at IISER Pune
13	Srita Dutta	Qualified CSIR-NET LS	2022	Research Fellow at TIFR
		and GATE		Hvderabad
14	Savantika Kar	Oualified GATE	2022	Research Fellow at IIT Kharagour
15	Nil Lohit	Qualified GATE	2022	Research Fellow at IIT Kharagpur
1.5	Sengupta	Zumined OTTL	2022	resource renow at itri Kharagpui
16	Sayan Bhadra	Qualified GATE	2022	Research Fellow at IIEST Shibpur
		(Rank-174)		

# Department of Chemistry, Bidhannagar College

Sl	Name of the	Achievement	Year	Current position
No	student			
17	Suman Majumder	Qualified CSIR-NET LS	2022	Yet to join
	Trisha	Qualified CSIR-NET JRF	2022	Research Fellow at IIT Madras
	Chakraborty			
18	Rakesh Halder	Qualified CSIR-NET JRF	2022	Research Fellow at IISER Kolkata
		(Rank- 141)		
19	Suman Sarkar	Qualified GATE	2022	Research Fellow at Central Salt and
				Marine Chemical Research
				Institute
20	Sayan Bhadra	Qualified CSIR-NET JRF	2023	Research Fellow at IIEST Shibpur
		(Rank- 55)		
21	Sampa Mondal	Qualified UGC-NET JRF	2023	Research Fellow at IIEST Shibpur
		(Rank- 119)		
22	Atanu Halder	Qualified GATE	2023	Research Fellow at IIT Madrass
23	Semanti Das	Qualified GATE	2023	Research Fellow at IICB, Kolkata
24	Binoy Ghosh	Qualified GATE	2023	Research Fellow at Jadavpur
				University
25	Shamim Molla	Qualified CSIR-UGC	2023	Research Fellow at IISER Bhopal
		NET LS		
26	Sandip Ghosh	Qualified CSIR-UGC	2023	Yet to join
		NET LS		
27	Arabinda Halder	Qualified GATE	2023	Yet to join

# **PG Syllabus**

# **Course structure:**

Semester I		
CHEMCOR01: Inorganic Chemistry – 1		50M
Unit 1: Symmetry and point group	13M	
Unit 2: Coordination chemistry	12M	
Unit 3: Solid state chemistry	13M	
Unit 4: Electrochemical analysis	12M	
CHEMCOR02: Organic Chemistry – 1		50M
Unit 1: Stereochemistry	13M	
Unit 2: Reaction mechanism and Methods of determination	12M	
Unit 3: Pericyclic Reactions	13M	
Unit 4: NMR spectroscopy	12M	
CHEMCOR03: Physical Chemistry – 1		50M
Unit 1 : Quantum Mechanics-I	13M	
Unit 2 : Electrochemistry - I	12M	
Unit 3 : Chemical Kinetics-I	13M	
Unit 4 : Spectroscopy	12M	
CHEMCOR04: Practical – 1		50M
(A) Inorganic Chemistry Practical:	30M	
Synthesis, complexometric and spectrophometric estimation		
(B) Physical Chemistry Practical - I	20M	
CHEMCOR05: Practical – 2		50M
Organic Chemistry Practical		
(A) Systematic qualitative analysis of a liquid organic compound	30M	
(B) Purification and drying of organic solvents	10M	
(C) Extraction and purification of organic compound from natural source	10M	
CHEMAEC01		50M

Computer operations for chemical science

# Semester II

CHEMCOR06: Inorganic Chemistry – 2		50M
Unit 1: Chemical bonding	13M	
Unit 2: Chemistry of s and p block elements	12M	
Unit 3: Chemistry of d block elements	13M	
Unit 4: Organometallic chemistry I	12M	
CHEMCOR07: Organic Chemistry – 2		50M
Unit 1: Synthetic methodology:	13M	
i) organoboron ii) organosulfur iii) organosilicon		
Unit 2: Heterocyclic chemistry	12M	
Unit 3: Synthetic strategy:	13M	
i) target oriented synthesis ii) method oriented synthesis		
Unit 4: Natural products	12M	
CHEMCOR08: Physical Chemistry – 2		50M
Unit-1: Mathematics for Chemistry and Quantum Mechanics II	13M	
Unit-2: Chemical Kinetics-II	12M	
Unit-3: Statistical Thermodynamics I	13M	
Unit 4: Group Theory	12M	
CHEMCOR09: Practical – 3		50M
Inorganic Chemistry Practical		
(A) Qualitative analysis including rare elements	25M	
(B) Analysis of ores, minerals and alloys	25M	
CHEMCOR10: Practical – 4		50M
(A) Organic Chemistry Practical Purification and identification of organic compounds in binary n	30M	
(B) Physical Chemistry Practical - II	10M	
	10141	
(C) Lab Quiz (Inorganic + Organic + Physical)	10M	
CHEMSEC01		50M
Chemical and spectral analysis		

# Semester III

CHEMCOR11: Inorganic Chemistry – 3		50M
Unit 1: Bio-inorganic Chemistyry I	13M	
Unit 2: Nuclear Chemistry and Radiochemical analysis	12M	
Unit 3: Chemistry of f-block elements	13M	
Unit 4: Complex equilibria	12M	
CHEMCOR12: Organic Chemistry – 3		50M
Unit 1: Photochemistry and Radical reactions	13M	
Unit 2: Organotransition metal chemistry	12M	
Unit 3: Oxidation Reduction and some special reactions	13M	
Unit 4: Advanced heterocyclic chemistry	12M	
CHEMCOR13: Physical Chemistry – 3		50M
Unit-1: Quantum Mechanics III	13M	
Unit-2: Nanomaterials	12M	
Unit-3: Statistical Mechanics II	13M	
Unit-4: Electrochemistry II	12M	
CHEMCOR14: Practical – 5		
Physical Chemistry Practical		50M
CHEMDSE01: ELECTIVE		50M
Spectroscopy		
Unit 1: Mass & IR spectroscopy	13M	
Unit 2: Emission Spectroscopy	12M	
Unit 3: Mossbauer spectroscopy & Photoelectron spectroscopy	13M	
Unit 4: Electron spin resonance spectroscopy	12M	
Analytical Chemistry		
Unit 1: Fundamentals of Chemical Analysis	13M	
Unit 2: Solvent Extraction and Concept of Chromatography	12M	
Unit 3: Liquid Chromatography and Other Types of Chromatography	13M	
Unit 4: Kinetics in Analytical Chemistry & Thermal Analysis	12M	
GEC: Basic Thermodynamics, Spectroscopy and Essence of Biochemi	stry (for other di	sciplines) 50M
Unit 1: Thermodynamics	13M	501/1

Unit 1: Thermodynamics	13M
Unit 2: Spectroscopy – I	12M
Unit 3: Spectroscopy – II	13M
Unit 4: Bioorganic and Bioinorganic Chemistry	12M

Semester IV		
CHEMCOR15: Inorganic Chemistry – 4		50M
Unit 1: Magnetochemistry	13M	
Unit 2: Inorganic ring, cages and clusters	12M	
Unit 3: Organometallic chemistry II	13M	
Unit 4: Chemical application of group theory	12M	
CHEMCOR16: Organic Chemistry – 4		50M
Unit 1: Asymmetric Synthesis	13M	
Unit 2: Medicinal Chemistry	12M	
Unit 3: Supramolecular Chemistry	13M	
Unit 4: Natural Products (Biosynthesis)	12M	
CHEMCOR17: Physical Chemistry – 4		50M
Unit-1: Quantum Mechanics and Spectroscopy	13M	
Unit-2: Material Chemistry	12M	
Unit 3: Laser and advanced Photophysics	13M	
Unit-4: Bio-physical Chemistry	12M	
CHEMDSE02 – Elective		50M
Inorganic Chemistry		
Unit 1: Advanced bio-inorganic chemistry	13M	
Unit 2: Spectroscopic analysis of inorganic compounds	12M	
Unit 3: Inorganic reaction mechanism	13M	
Unit 4: Crystallography	12M	
Organic Chemistry		
Unit 1: Advanced Stereochemistry	13M	
Unit 2: Advanced Pericyclic Reactions	12M	
Unit 3: Advanced NMR spectroscopy	13M	
Unit 4: Molecules of life	12M	
Physical Chemistry		
Unit-1: Advanced Quantum Mechanics	13M	
Unit 2: Non-equilibrium thermodynamics	12M	
Unit 3: Macromolecules	13M	
Unit 4: Statistical Mechanics III	12M	
CHEMDSE03 – Laboratory Experiment & Research Project		100M
Unit 1: Laboratory Experiment	25M	
Inorganic: Physico-chemical experiment;		
Organic: Multistep organic synthesis		
Physical: Spectrophotometric experiment		
Unit 2: Project work	30M	
Unit 3: Literature Review	30M	
Unit 4: Grand Viva	15M	

# **Detailed syllabus:**

#### Semester I

#### CHEMCOR01: Inorganic Chemistry – 1 [Credits – 4]

#### Unit 1: Symmetry and point group

The concept of groups, subgroups, classes and the related theorems; Group multiplication tables and the rearrangement theorem. Symmetry elements and operations, products of symmetry operations, identification of point groups, Hermann-Mauguin (HM) notations; similarity transformation, block diagonalisation; Matrix representation of symmetry operations, characters of symmetry operations in a row / column orthogonality of characters, reducible and irreducible representation, the representations, the "Great Orthogonality Theorem" (without derivation) and Standard reduction formula.

#### **Unit 2: Coordination Chemistry**

Crystal Field Theory: Spitting of d orbitals in crystal fields of different symmetry for similar and dissimilar ligands, Thermodynamic aspects of crystal field splitting, Kinetic aspects of crystal field stabilization: crystal field activation energy, labile and inert complexes.

Electronic spectra of transition metal complexes: Microstates, determination of ground and excited state terms of d<sup>n</sup>ions; Orgel diagrams (qualitative approach), selection rules for spectral transitions, d-d spectra of d<sup>n</sup>ions and crystal field parameters, nephelauxetic series. Metal-ligand bonding (pictorial MO approach): sigma and pi-bonding in complexes, CT transitions.Crystal field splitting of free ion terms in weak and strong crystal fields ( $O_h$  and  $T_d$ ), energy level diagrams and symmetries and multiplicities of energy levels in strong crystal fields, Construction of mo diagrams of polyatomic molecules including coordination complexes ( $O_h$  and  $T_d$ ), sandwich complexes: (ferrocene, dibenzenechromium).

Magnetic properties of coordination compounds: spin and orbital moment, spin-orbit coupling, quenching of orbital moment, spin only formula.

#### **Unit 3: Solid state Chemistry**

Defects in solids, Point, Line and Plane defects, Determination of equilibrium concentration of Schottky and Frenkel defects, Stoichiometric imbalance in crystals and non-stoichiometric planes, colors centers in ionic crystals, band theory, band gap, metals, insulators, semiconductors(intrinsic and extrinsic), hopping semiconductor, rectifiers and transistors.

#### **Unit 4: Electrochemical analysis**

Basic principle, instrumentation, special futures and applications in inorganic analysis (Qualitative/quantitative as applicable) of the following techniques

Electroanalytical methods: Polarography: Ilkovic equation, half wave potential and its significance. Ampherometric titration, Coulometry, cyclic voltametry, ion selective electrode, electrogravimetry.

#### 12M

**13M** 

#### 12M

# **13M**

#### CHEMCOR02: Organic Chemistry – 1 [Credits – 4]

#### **Unit 1: Stereochemistry**

Static Aspects: symmetry properties, point groups, streoisomerism with asymmetric carbons in branched chains, nomenclature:  $R^*/S^*$ , racemate, polysubstituted cyclane, molecules with a centre of chirality and simple axes of symmetry, stereoheterotopic ligands and faces, axial chirality, planar chirality and helicity. Conformational analysis of cyclic system (cyclohexene, cyclohexanone, substituted cyclopentanes and cyclopentanes, medium rings, decalin and hydrindane systems)

Dynamic Aspects: conformation and reactivity with reference to substitution, elimination, addition and rearrangement reactions. Winstein-Holness equation. Curtin Hammett principle.

#### Unit 2: Reaction mechanism and methods of determination

Types, intermediates, thermodyanamic and kinetic requirements, Hammond postulate, microscopic reversibility.

Methods: Identification of products, Isotope labeling, Intermediates, catalysis, kinetic methods, isotope effects, stereochemical course of the reaction.

Correlation of structure and reactivity: Hammett equation, Substituent constant, reaction constant, physical significance, use of Hammett plot – reaction mechanism and picture of transition state; nonlinear Hammett plots.

#### **Unit 3: Pericyclic reactions**

Molecular orbitals for acyclic conjugated systems. Theory of pericyclic reactions – i) Frontier Molecular Orbital (FMO) approach ii) concept of aromaticity of transition states (Hückel / Möbius systems). The Woodward-Hoffmann selection rules and general rules. Scope, reactivity and stereochemical features of electrocyclic reactions (4e, 6e and 8e neutral systems), cycloaddition reactions ([4+2] and [2+2]), cheletropic reactions and signatropic rearrangements ([1,3] and [1,5] shifts, [1,7] H shift, [3,3] rearrangements), group transfer reactions.

#### Unit 4: NMR spectroscopy

<sup>1</sup>H NMR Spectroscopy: Equivalence and nonequivalence of protons, spin-spin coupling – notation for spin systems, coupling constant and its variation with stereochemistry – Karplus equation.

<sup>13</sup>C NMR Spectroscopy: Principles; broad band coupling.

Application of <sup>1</sup>H NMR and <sup>13</sup>C NMR for structure elucidation.

#### CHEMCOR03: Physical Chemistry – 1 [Credits – 4]

#### Unit 1: Quantum Mechanics-I

Postulates of quantum mechanics and their analysis; Properties of operators and commutators; Timeindependent Schrodinger equation; Concept of stationary states, Free particle, Particle in a one dimensional box, Barrier problems and tunnelling phenomenon ; Equation of motion; Ehrenfest's theorems, Role of the constant of motion. Angular momentum operators, Eigenvalues and eigenfunctions, Hydrogen atom Problem: Cartesian and Polar coordinates. Centre of Mass and relative coordinate, Spherical harmonics. Real and complex orbital.

#### Unit 2 : Electrochemistry I

Ion-Ion interaction: Debye Huckel theory and its extension. Electrode kinetics: Nernst, Butler-Volmer equation, Tafel equation. Overpotential. Fuel cells. Corrosion and its control.

# 13M

12M

### 50M 13M

#### 12M

### 50M 13M

#### Unit 4: Spectroscopy General introduction

**Unit 3: Chemical Kinetics-I** 

mechanism. Autocatalytic reaction.

General introduction, nature of electromagnetic interaction, shapes and width of spectral lines, intensity of spectral lines, Fourier transform, Microwave spectroscopy : Moment of inertia and classification of molecules, Energy expression for symmetric rotor. Stark Effect and determination of Dipole moment. Non-rigid rotor, Breakdown of Born-Oppenheimer approximation, vibrational-rotational spectra

### CHEMCOR04: Practical – 1 [Credits – 4]

### (A) Inorganic Chemistry Practical:

Synthesis, complexometric and spectrophometric estimation

Synthesis of some metal complexes:

*tris*(ethylenediamine)nickel(II) thiosulphate, *tris*(acetylacetonato)manganese(II), hexaminecobalt(III) chloride, mercury tetrathiocyanatocobaltate(II), Reinicke's salt, *bis*(biguanido) copper(II) sulphate. Complexometric Estimation:

Fe(III) and Al(III) in a mixture, Cu(II) and Zn(II) in a mixture.

Spectrophotometric Determination of:

i) Fe(III) by sulphosalicylic acid and thiocyanate methodii) Mn(II) by periodate oxidation method

## (B) Physical Chemistry Practical - I

1. Determination of thermodynamic Solubility Product of  $PbI_2$  in water at room temperature.

2. Determination of Standard Reduction Potential ( $E^{\circ}$ ) of the Quinhydrone electrode by potentiometric method

3. Determination of Hydrolysis Constant of a Salt with the Help of a pH-meter

4. Conductometric titration of a Mixture of Halides (KCl + HCl + NH<sub>4</sub>Cl) by i) NaOH and ii) AgNO<sub>3</sub>

5. Determination of Critical Micelle Concentration (CMC) of SDS conductometrically.

6. Determination of acidic and basic dissociation constant of amino acid (glycine) and hence determination of its isoelectric point.

CHEMCOR05: Practical – 2 [Credits – 4]	50M
Organic Chemistry Practical	
(A) Systematic qualitative analysis of a liquid organic compound	30M
(B) Purification and drying of organic solvents	10M
(C) Extraction and purification of organic compound from natural source	10M

## CHEMAEC01: [Credits – 2]

Computer operations for chemical science

Collision theory and activated complex theory. Reactions between ions: influence of solvent dielectric constant (double sphere model), single sphere activated complex model, influence of ionic strength. Effect of pressure on rate constant: Concept of volume of activation. Unimolecular reactions: Lindemann-Hinshelwood mechanism and RRK mechanism. Chain reactions. Oscillatory reactions: Observation and

#### 12M

**50M** 

**30M** 

**13M** 

**50M** 

#### Semester II

#### CHEMCOR06: Inorganic Chemistry – 2 [Credits – 4]

#### Unit 1: Chemical bonding

LCAO-MO and VB treatments on  $H_2^+$ ,  $H_2$ ; application to homo- and hetero- nuclear diatomic molecules/ ions of second period elements, electron density, forces and theirrole in chemical bonding. Hybridization and valences, MO's of  $H_2O$ ,  $NH_3$ ,  $CH_4$ .Huckel – pi – electron theory and its applications to ethylene, butadiene and benzene, idea of self consistent field. Concept of resonance.

#### Unit 2: 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, cryptates and spherand). Aqueous and complex chemistry of beryllium and aluminium. Main group organometallic chemistry: classification, synthesis, reaction, structure and bonding, and application of typical examples.

#### Unit 3: Chemistry of d block elements

Electronic configuration, oxidation states; aqueous, redox and complex chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d, 4d and 5d elements with references to Ti-Zr-Hf, Cr-Mo-W, Mn-Tc-Re and Pt group metals. Mixed valence compounds of Fe, Cu, Pt; Fe-S compounds, cobaloxime related compounds, conformational changes and thermochromism of Ni(II) compounds, Ru(II) and Ru(III) compounds, oxo compounds of Ru and Os, Rh(I) and Ir(I) carbonyl halide and carbonylhydrides.

Synthesis, properties, reactions, structure and bonding as applicable in respect of: Mo-blue, W-blue, Pt-blue, W-bronze, Ru-red, Creutz- Traube complexes, Vaska's complexes.

Iso- and hetero metallates derived from V, Mo and W (synthesis, structure and applications).

#### Unit 4: Organometallic Chemistry I

*Main group organometallics:* Classification, synthesis, reactions, structure and bonding and applications with typical examples. Application of 18- electron and 16- electron rules to transition metal organometallics, structure, bonding (pictorial mo-approach) and reactions of of  $\eta$ 2-ethylinic ,  $\eta$ 3-allylic and  $\eta$ 5- cyclopentadineyl compounds: K [ Pt ( $\eta$ 2 -C2H4)Cl3], [( $\eta$ 3-C3H5) Pd Cl ]2, ( $\eta$ 5- C5H5)2 Fe]; carbene and carbyne complexes. Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

#### CHEMCOR07: Organic Chemistry – 2 [Credits – 4]

#### **Unit-1: Synthetic Methodology**

Organoboron: Hydroborations; Reduction; Reactions of organoboranes; Unsaturated hydrocarbon synthesis; Allyl borane and boron enolates.

Organosulphur:Sulphur stabilization of anions and cations, Sulphonium salts, Sulphonium and sulphoxonium ylides

Organosilicon:Alkene synthesis, Alkenyl, Vinyl, Aryl, Allyl and Acylsilanes; Brook rearrangement; Silicon Baeyer-Villiger rearrangement.

### 12M

#### 50M

**13M** 

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12M

#### Unit-2: Heterocyclic Chemistry:

Systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles; heterocycles in organic synthesis-Masked functionalities, umpolung, Storkamination reation, rearrangement and ring transformation involving 5-, 6- memberedheterocycles with one hetero atom, general approach to heterocycle synthesis, cyclisation,cycloaddition route.

#### **Unit-3: Synthetic strategy:**

i) Target-oriented synthesis – natural products, designed molecules
ii) Method oriented synthesis – reagents, catalysts, synthetic strategies and tactics.

#### **Unit-4: Natural Products**

Structural types; structure elucidation, reactions and synthesis of representative examples of (i) Alkaloids [coniine, tropines, cocaine, quinine] (ii) Terpenoids [pinene, camphor, caryophyllene] (iii) Steroids [cholesterol]

#### CHEMCOR08: Physical Chemistry – 2 [Credits – 4] 50M

#### Unit-1: Mathematics for Chemistry and Quantum Mechanics II

Elements of calculus, Extremum principles, constrained extremization, Power series: Convergence and divergence, Taylor series and Fourier series. Vectors and linear vector space: matrices. Applications. Particle on a ring, Rigid Rotor, Ladder operators; Harmonic Oscillator, Calculation of various quantities (matrix elements, selection rule, etc) using ladder operators and recursion relations of Hermite polynomials. Variation theorem and variational methods. Use of these methods illustrated with some examples (anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

#### **Unit-2: Chemical Kinetics-II**

Different types of mechanism of enzyme catalysed reactions. Influence of pH, temperature and inhibitors on such reactions. Surface reactions. Micelles, Micellar catalysis and its application. Kinetics of fast reactions: flow method, relaxation method, flash photolysis. Diffusion controlled reaction and its kinetics.

#### **Unit-3: Statistical Thermodynamics I**

Entropy and Probability; Ensembles-Types; Partition Function and Thermodynamic properties; Maxwell Boltzmann distribution. The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases ; Calculation of thermodynamic properties of ideal gases in terms of partition function. Calculation of equilibrium constants of gaseous solutions in terms of partition function, Application to chemical/ionization equilibrium.

#### **Unit 4: Group Theory**

Matrix representations, great orthogonality theorem and its consequences; character table. Symmetry adapted linear combination (SALC) with illustrative examples. Construction of Molecular Orbitals using Huckel approximation.

#### 12M

**13M** 

# 12M

#### 12M

12M

**13M** 

CHEMCOR09: Practical – 3 [Credits – 4]	50M
Inorganic Chemistry Practical	50M
(A) Semimicro qualitative inorganic analysis including rare elements 25M Semi-Micro Qualitative Inorganic Analysis of Complex Inorganic Mixtures containingnot mo (6) inorganic radicals from the lists ( <i>a</i> ), ( <i>b</i> ), ( <i>c</i> ), and ( <i>d</i> ), of which two(2) radicals must be derived rare elements ( <i>d</i> ), and the mixture should notcontain more than one insoluble material from the and ( <i>d</i> ) : ( <i>a</i> ). Cation Radicals derived from:Ag, Hg, Pb, Bi, Cd, Cu, As, Sb, Sn, Fe, Al, Cr, Co, Ni, Mn, Z Ca,Mg, Na, K and NH <sub>4</sub> <sup>+</sup> ion. ( <i>b</i> ). Anion Radicals: F <sup>-</sup> , Cl <sup>-</sup> , Br <sup>-</sup> , I <sup>-</sup> , BrO <sub>3</sub> <sup>-</sup> , IO <sub>3</sub> <sup>-</sup> , SCN <sup>-</sup> , S <sup>2-</sup> S2O <sub>3</sub> <sup>2-</sup> , SO <sub>4</sub> <sup>2-</sup> , NO <sub>2</sub> <sup>-</sup> , NO <sub>3</sub> <sup>-</sup> , PO <sub>4</sub> <sup>3-</sup> 'AsO <sub>4</sub> <sup>3-</sup> , BO <sub>3</sub> <sup>3-</sup> , H <sub>3</sub> BO <sub>3</sub> ,SiO <sub>2</sub> <sup>-</sup> ,CrO <sub>4</sub> <sup>2-</sup> , Cr <sub>2</sub> O <sub>7</sub> <sup>2-</sup> , [Fe(CN) <sub>6</sub> <sup>4-</sup> ], [Fe(CN) <sub>6</sub> <sup>3-</sup> ]. ( <i>c</i> ). Insoluble Materials:PbSO <sub>4</sub> , BaSO <sub>4</sub> , SrSO <sub>4</sub> , PbCrO <sub>4</sub> , CaF <sub>2</sub> , SiO <sub>2</sub> and various silicates, SnO <sub>2</sub> Fe <sub>2</sub> O <sub>3</sub> , Cr <sub>2</sub> O <sub>3</sub> , AgCl, AgBr, AgI. ( <i>d</i> ). Cation radicals, anion radicals and insoluble materials derived from the followingrare Eleme Mo, W, U, Ti, Zr and Ce. Experiment-1: Known tests for detection of radicals derived from rare elements. Experiment-2: Treatment of known insoluble materials. Experiment-3: Analysis of unknown inorganic mixtures containing six radicals includingtwo rad derived from the rare elements (at least 4-5 samples)	are than six ad from the he lists <i>(c)</i> , Zn, Ba, Sr, $(AsO_3^{3-})$ , $Al_2O_3$ , ents: V, dicals
(B) Analysis of ores, minerals and alloys 25M <i>Ores, Minerals</i> :Dolomite (CaCO <sub>3</sub> , MgCO <sub>3</sub> , Fe <sub>2</sub> O <sub>3</sub> , SiO <sub>2</sub> ); Pyrolusite (MnO <sub>2</sub> , MnO, Fe <sub>2</sub> O <sub>3</sub> ); Ch (CuS, FeS); Bauxite (Al <sub>2</sub> O <sub>3</sub> , Fe <sub>2</sub> O <sub>3</sub> , TiO <sub>2</sub> , SiO <sub>2</sub> ). <i>Alloys</i> :Brass (Cu, Zn); Bronze (Cu, Zn, Sn), Steel (Cr, Mn, Ni, P), Type metal (Pb, Sb, Sn).	nalcopyrite
CHEMCOR10: Practical – 4 [Credits – 4]	50M
Organic Chemistry Practical	30M

Separation, purification and identification of organic compounds in binary mixtures (two solids, two liquids and one solid + one liquid) using solubility method & chromatographic method and systematic qualitative analysis by chemical & spectroscopic (UV, IR, NMR) techniques.

#### **Physical Chemistry Practical II**

1. Potentiometric Titration of (KI+KBr) by AgNO<sub>3</sub> solution.

2. Kinetic study of the autocatalytic reaction between potassium permanganate and oxalic acid.

3. Verification of the Onsager equation and Conductometric determination of Solubility Product of a sparingly soluble salt.

4. pH-metric titration of a polybasic acid and determination of its basicity and dissociation constants

Lab Quiz (Inorganic + Organic + Physical)

**10M** 

#### CHEMSEC01: [Credits – 2]

#### Chemical and spectral analysis

(1) Elucidation of different methods of synthesis and characterization of inorganic and coordination compounds-some representative examples:

A. Polynuclear clusters reported in literature.

B. Mn<sub>12</sub> Acetate.

C. Preparation of copper glycine complex-bis(glycinato)copper (II).

D. Preparation of N,N-bis(salicyldehyde)ethylenediamine, Co(salen)

E. Selected coordination compounds with some common inorganic and organic ligands and with

bi-, tri- and polydentate N, O donor ligands, oximes etc; Complexation and purification of complexes; estimation of metal inos present in coordination complexes

#### (2) Parameters of water analysis

Procedure of analysis of BOD, COD, DO, TOC, TOD and similar parameters

#### (3) Spectroscopic analysis:

Basic idea of using UV, IR, NMR, MASS, ESR spectrometry and elemental analysis:

Determination of empirical formula from elemental analysis, Determination of molecular formula using molecular mass of the compound, Systematic application of the spectral data to determine and confirm the structure of the molecule by interpreting the supplied and/or obtained spectral data, Application of the spectra to study and diagnose various molecular properties.

#### Semester III

#### CHEMCOR11: Inorganic Chemistry – 3 [Credits – 4]

#### Unit 1: Bio-inorganic Chemisty I

Essential and trace elements in the biological systems, metal of life, basic reactions in the biological systems and the roles of metal ions in biological process. Bioenergetic principle: ATP-ADP inter conversion.

Oxygen transport and storage proteins: Active site structures and biofunctions ofhemocyanin and hemerythrin; synthetic dioxygen complexes as models.

Biological redox couples:  $NAD^+/NADH$  and  $NADP^+/NADPH$ ,  $FAD/FADH_2$ , ubiquinone and plastoquinone.

Photosynthesis and chlorophylls, photosystem (PS)-I, photosystem (PS)-II and their roles in cleavage of water, model systems. Biological nitrogen fixation: nitrogenase enzyme complex and mechanism of its action, model abiological nitrogen fixation systems.

Toxic effects of metal ions, detoxification by chelation therapy, metal dependent diseases: Wilson's disease, Alzheimer's disease; metal complexes as drugs: Pt, Rh, Ru and Au drugs.

#### Unit 2: Nuclear Chemistry and Radiochemical analysis

*Nuclear models:* Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism.

50M 13M

Nuclear reactions: Nuclear reactors and particle accelerators, energetics of nuclear reactions, Q-value, nuclear cross-section, mechanism and models of nuclear reactions. Nuclear fission and nuclear fusion, fission products and fission yields. Interactions of radiation with matters, chemical effects of nuclear transmutation (elementary idea), radiolysis of water and other liquids/ solutions.

Radioactive techniques: Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

#### Unit 3: Chemistry of f-block elements

*f*–*BlockElements*:LanthanideandActinideElements:

Nuclearstability, terrestrialabundance, distribution. relativistic effect, electronic configuration, oxidation states, aqueous-, redox-and complex-chemistry; electronic spectra and magnetic properties. Lanthanide and actinide contractions and their consequences, separationof lanthanidesandactinidesand theirapplications(examples). Compounds of Sc, Y, Laand Ac;Ce(III) and Ce(IV) compounds and their reactions, Lanthanide compounds as high temperature superconductor, nmr shiftreagentand MRI reagent.

#### **Unit 4: Complex equilibria**

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

CHEMCOR12: Organic Chemistry – 3	Credits – 41	50	Μ
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#### **Unit 1: Photochemistry and Radical reactions**

#### **Photochemistry**

Basic principles, Jablonski diagram, Direct and sensitized reactions, Photochemistry of olefinic compounds; cis-trans isomerisation; Patterno-Buchi reaction; Norish type-I and Norish type-II reaction; Photo-reduction of ketone; Di-pi methane rearrangement.

#### **Radical reactions**

Radicals and their synthetic uses, Bonding and preferred geometries, generation, stability (reactive and unreactive radicals), radical initiators, defunctionalisations, radical addition and fragmentation reactions: C - X bond, C - C bond forming reactions, C - C bond cleaving reactions.

#### **Unit 2: Organotransition metal Chemistry**

Organometallic reaction mechanism; Homogeneous hydrogenation; Organometallics as electrophiles; Synthetic applications of transition metal alkene complexes, Synthetic applications of complexes containing metal – carbon  $\sigma$  bonds: Heck and related reactions, carbonylation reactions; Synthetic applications of transition metal carbene complexes: Fischer carbene, Schrock carbene, metathesis processes, Tebbe's reagent, Zieglar - Natta reaction; Synthetic applications of transition metal alkyne complexes, Applications of transition metal complexes in organic synthesis.

**13M** 

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#### Unit 3: Oxidation Reduction and some special reactions

One electron and two electron oxidants, Oxidations with Cr (VI): Jones oxidation, Collins oxidation PCC, PDC, PFC; DMSO based oxidations: Swern, Moffat, DMSO-SO<sub>3</sub> complex, DMSO-acetic anhydride, Hypervalent iodine oxidations: Dess-Martine periodinane, IBX, Iodobenzene diacetate; Oxidations with thalium nitrate, Ag<sub>2</sub>O, RuO<sub>4</sub>, OSO<sub>4</sub>, NaIO<sub>4</sub>. Reduction with metal-hydrides of B, Al, Sn, Si. Dissolving metal-reduction, Synthetically useful hydrogenolysis reaction, Sm and In based reducing agents and enzymatic reductions.

Shapiro reaction, Mitsunobu reaction, Hofmann-Loffler-Freytag reaction, Barton reaction, Barton decarboxylation and deoxygenation reaction, Tandem cycloaddition reaction, Baylis - Hilman Reaction, Passerini reaction, Ugi Reactions

#### Unit 4: Advanced heterocyclic chemistry

Synthesis and reactions of aziridines, azitidines, oxazoles, thiazoles, imidazoles, isoxazoles, isothiazoles, pyrazoles and higher azoles and corresponding few systems, pyrimidines, pyridazines, pyrazines, purines, pteridines, role of heterocyclic compounds in biological systems, nomenclature of bicyclic and tricyclic fused systems, Introduction to the chemistry of azipines, oxepins, thiepins and their aza-analouges, cyclazines.

#### CHEMCOR13: Physical Chemistry – 3 [Credits – 4]

#### Unit-1: Quantum Mechanics III

Rayleigh-Schrodinger perturbation theory for non-degenerate states with simple applications, Degenerate perturbation theory, Stark effect, First and second order lifting of degeneracy.

Time-dependent perturbation theory, Derivation of Fermi's golden rule, Harmonic perturbation and transition probabilities.

#### **Unit-2: Nanomaterials**

Nanomaterial- definition, classification and properties, relevance to dependency on size and shape. Synthetic methodologies both physical and soft chemical methods { i) mechanical methods, ii) Evaporation methods, iii) CVD, iv)Sol-gel, v) Micromulsion (normal and reverse micelles formation), vi) Template based synthesis, vii) reduction methods }. Various kind of Nanostructures; Quantum dot (QDs), Carbon Nanotubes, (SWCNT, MWCNT), Fullerene, Graphene, etc.Nanotechnology. Application of nanomaterials and nanotechnology. Biomedical applicaton – drug delivery, advantages and limitations.

#### **Unit-3: Statistical Mechanics II**

Phase space, ergodic hypothesis, Liouville's theorem, Concepts of different ensembles with applications to selective systems. Fluctuations. Perfect gas and the Sackur-Tetrode equation, System of interacting molecules, treatment of imperfect gases, Black body radiation.

#### **Unit-4: Electrochemistry II**

Ion-transport in solution: Debye-Huckel-Onsager theory and its extension. Electrode surface: Potential and measurements, Thermodynamics of such system, Lippmann equation, surface excess and its determination from electrocapillary measurements. Structure of Double layer: Helmholtz- Perrin, Gouy-Chapman and Stern and Contact adsorption model.

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#### CHEMCOR14: Practical – 5 [Credits – 4]

Physical Chemistry Practical

1. Kinetic Study of the reaction between  $K_2S_2O_8$  and KI and study on the effect of added salt on the rate constant.

2. Study of the ternary phase diagram of glacial acetic acid, water and benzene at room temperature and atmospheric pressure.

3. Determination of the Standard Electrode Potential (E°) of Ag/Ag+ system and Activity Coefficient of Ag+ ions in solution.

4. Studies on Kinetics of Iodination of Acetone.

5. Study of the determination of the decomposition of hydrogen peroxide by acidified KI, maintaining a constant excess of iodide. Determination of the rate constant at four different temperatures and hence determination of the energy of activation, enthalpy of activation and entropy of activation of the reaction.

6. Determination of Isoelectric Point of a protein (Gelatine) by Ostwald viscometer.

7. Determination of equilibrium constant of acid hydrolysis of an ester.

8. Determination of the formula of silver amine complex.

9. Potentiometric titration of acetic acid by sodium hydroxide using quinhydrone electrode.

10. Determination of individual strengths of (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> and Na<sub>2</sub>SO<sub>4</sub> in their mixture conductometrically.

#### CHEMDSE01: ELECTIVE [Credits – 4]

#### Spectroscopy

#### Unit-1: Mass & IR spectroscopy

Mass spectroscopy: Basic instrumentation, ion production - EI,CI, FD and FAB techniques, Mass spectral fragmentation of typical organic compounds, common functional groups.

IR spectroscopy: Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic and heterocyclic compounds, ethers, phenols and amines, carbonyl compounds (aldehydes, ketones, esters, carboxylic acids, amides, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effects of solvent, hydrogen bonding on vibrational frequencies, overtones, combination bands and Fermi resonance, FT IR.

#### **Unit-2 : Emission spectroscopy**

Franck-Condon principle, Mirror-image symmetry and its violation, Radiative and radiationless deactivation, Oscillator strength, Fluoroscence Quenchers and life-time variations, Photophysical processes of unimolecular processes, Delayed fluorescence, Kinetics of bimolecular processes: collision quenching, Stern-Volmer equation, Concentration dependence of quenching and excimer formation, Excited state electron transfer processes.

#### Unit-3: Mossbauer spectroscopy & Photoelectron spectroscopy

Principle, experiment, line-width center shift, quadrupole interaction, magnetic interaction, information of spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in varieties of environments Photo excitation and photoionization, core level photo ionization (XPS, ESCA.) and valence level (UPS) experiments, detection of atoms in molecules, chemical shift, differentiating same element in different environments.

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### Unit-4: Electron spin resonance spectroscopy

Basic principles, Principle of EPR and spin Hamiltonian (comparison to NMR spectroscopy), external standard, line-width, nuclear hyperfine interactions, anisotropy in Lande g factor and hyperfine interaction, zero field splitting, and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities. Basic instrumentation, measurement techniques and simple applications regarding structural information of organic radical and inorganic molecules from EPR spectra.

### Analytical Chemistry

### Unit-1: Fundamentals of Chemical Analysis

Aim of analytical chemistry. Standardization and calibration. Quality assurance and quality control. Process control and validation.

Classical methods of analysis: Gravimetry and titrimetry including neutralization, complexationand oxidation-reduction. Complex acid-base equilibrium. Separation of metal ions as theirhydroxides, sulphides and chelates. Examples of gravimetric and complexometric analysis.

### Unit-2: Solvent Extraction and Concept of Chromatography

Liquid-Liquid extraction – Cross and counter current process, multiple batch extraction, solvent extraction of metal ion, solid-phase extraction. Classification of chromatographicseparation. Aqueous biphasic and supercritical fluid extraction. Band broadening and columnefficiency, Theoretical plate model and the Rate theory of Chromatography.

### Unit-3: Liquid Chromatography and Other Types of Chromatography: 13 M

Reverse and normal phase chromatography, gradient elution, solvent selection and classes, ion exchange and ion chromatography.

HPLC: Basic equipment, pumping and injection system, column stationary phase and structuraltypes of column packing, Detector systems (UV, IR, Conductometric, Fluorescence), Samplepreparation and applications.

Gas chromatography: gas-liquid and gas-solid chromatography, types of column and selection.

Basic equipment, Injection systems, Detectors (FID, TCD, ECD, NPD) for GC, sampleseparation and applications. Characteristics and applications of Size exclusionChromatography, Affinity chromatography, Supercritical Fluid Chromatography, CapillaryElectrophoresis.

### Unit- 4: Kinetics in Analytical Chemistry & Thermal Analysis

Significance of reaction kinetics in analytical chemistry. Determination of rate of fastreactions. Analytical application of catalytic and non-catalytic reactions in single species and pseudo single species systems. Differential reaction rate methods of analysis and its limitations, determination of inorganic and organic mixtures.

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#### GEC: Basic Thermodynamics, Spectroscopy and Essence of Biochemistry (for other disciplines) [Credits – 4] 50M

#### **Unit 1: Thermodynamics**

Brief resume of the concept of free energy, entropy and laws of Thermodynamics and general condition of equilibria. Dependence of thermodynamic functions of composition: partial molar quantities, their significance and methods of determination. Thermodynamic properties of gases with special reference to real gases in the pure state and in mixtures. Thermodynamics of ideal and non-ideal binary solutions, excess function for non-ideal solutions and their determination. Gibbs-Duhem equation applied to activity coefficient (Osmotic coefficient), Different scales of activity coefficients for solutes and solvents, Experimental determination of activity coefficients of electrolytes and non-electrolytes.

#### Unit 2: Spectroscopy – I

Nuclear magnetic resonance spectroscopy: Basic instrumentation, nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift, and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification of molecules: (ABX, AMX, ABC, A2B2, etc. types).

Application of UV & Vis spectroscopy, ORD & CD spectra, absolute configuration of chiral compounds.

#### Unit 3: Spectroscopy – II

**IR spectroscopy:** Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic and heterocyclic compounds, ethers, phenols and amines, carbonyl compounds (aldehydes, ketones, esters, carboxylic acids, amides, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effects of solvent, hydrogen bonding on vibrational frequencies, overtones, combination bands and Fermi resonance, FT IR.

Basic principles and simple applications of Raman Spectroscopy.

**Mass spectrometry:** Basic instrumentation, ion production - EI,CI, FD and FAB techniques, Mass spectral fragmentation of typical organic compounds, common functional groups.

#### Unit 4: Bioorganic and Bioinorganic Chemistry

**Bioorganic Chemistry:** Structure of proteins, classification of enzymes, co-enzymes, Mechanism in biological chemistry: mechanism of enzyme action, examples of enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidaseA

**Bioinorganic Chemistry:** Essential and trace elements in the biological systems, basic reactions in the biological systems and the roles of metal ions in biological process.

Ion transport across biological membrane and its significance, Na<sup>+</sup> pump and ionophores, Oxygen transport and storage proteins, hemoglobin, myoglobin.

Toxic effects of metal ions, detoxification by chelation therapy, metal dependent diseases, metal complexes as drugs.

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#### Semester IV

#### CHEMCOR15: Inorganic Chemistry – 4 [Credits – 4]

#### Unit 1: Magnetochemistry

Types of magnetic materials. Magnetic susceptibility and its determination: Gouy, Faraday and Evans methods, vibrating sample magnetometer, SQUID and NMR methods. Magnetic anisotropy, diamagnetism in atoms and polyatomic systems, Pascal's constants. Spin and orbital moments, spin-orbit coupling, Lande interval rule, energies of J states. Curie equation, Curies law and Curie-Weiss law. First order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of Van Vleck susceptibility equation. Quenching of magnetic moments of transition metal compounds in cubic and axially symmetric crystal fields, low spin- high spin crosser. Magnetic behaviour of Lanthanides and actinides; magnetic exchange interactions, magnetic materials.

#### Unit 2: Inorganic ring, cages and clusters

Metal-Metal bonding (M.O. Approach), metal-metalsingleandmultiplebondedcompounds. Low nuclearity (M3,M4) and high nuclearity (M5-M10) carbonyl clusters: skeletal electron counting,Wade-Mingos-Louherrule,Applicationofisolobalandisoelectronicrelationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

#### Unit 3: Organometallic chemistry II

Hydrogenation of olefins, Wilkinson's catalyst, Tolman Catalysis by Organometallic compounds: catalvtic loop: synthesis gas, water-gas shift reaction: Hvdroformvlation (oxo process),Monsantoaceticacidprocess,Wackerprocess;syntheticgasoline:Fischer-Tropsch process and Mobile process, polymerization, oligomerization and metathesis reactions of alkenes and alkynes, Zieglar-Natta catalysis, photo dehydrogenation catalyst (platinum POP).

#### **Unit 4: Chemical application of group theory**

Construction of character tables ( $C_2v$ ,  $C_3v$ ,  $C_4v$ ,  $D_4$ ), representation for cyclic groups, wave functions as bases for Irreducible Representations, symmetry of normal modes, normal mode analysis, selection rules for IR and Raman transitions. Projection operator (without derivation), use of the projection operator to form symmetry adapted linear combination (SALC) of simple system.

#### CHEMCOR16: Organic Chemistry – 4 [Credits – 4]

#### **Unit 1: Asymmetric Synthesis**

Principles; Use of chiral substrate, chiral reagent, chiral catalyst; Stereoselective reactions of carbonyl compounds: enolate formation, alkylation, asymmetric aldol reactions; Stereoselective reactions of alkenes: Diels-Alder reaction, sigmatropic rearrangement, stereoseletive hydrogenation, epoxidation, hydroxylation, aminohydroxylation, cyclopropanation; Kinetic resolution; Asymmetric synthesis of menthol (Takasago), crixivan (Merck)

#### **Unit 2: Medicinal Chemistry**

Bacterial and animal cells, antibacterial agents – mechanism with reference to  $\beta$ -lactam antibiotics, General method of synthesis of  $\beta$ -lactam ring: synthesis of penicillin, structure-activity relationship of penicillin.

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Synthesis and mechanism of action of (i)fluoroquinolones – norfloxacin, ciprofloxacin, levofloxacin (ii) anti AIDS drugs – AZT, lamivadine (iii) antihypertensive agent – captopril (iv) calcium channel blocker – amlodipine (v) gastric secretion inhibitor – omeprazole (vi) drug for impotency – sildenafil. Vitamins: vitamin B complex, vitamin-C, vitamin-K, Prostaglandins- structure and synthesis.

#### Unit 3: Supramolecular Chemistry

Molecular to supramolecular chemistry: Factors leading to strong binding (non-covalent interation), New molecular receptors, Crown ether, Siderophore, Cyclophanes, Cyclodextrin and their application in specific recognition processes, supramolecular reactivity and catalysis, Liquid crystals and supramolecular polymers; supramolecular devices: Electronic, ionic and switching devices; supramolecular sensors; Self assembling, self replication of supramolecular aggregates and auto-catalysis.

#### **Unit 4: Natural Products (Biosynthesis)**

Primary and secondary metabolites, biogenetic hypothesis, elucidation of biosynthetic pathways. Biosynthesis of terpenoids and steroids; Shikimic acid pathway: Biosynthesis of flavonoids; Biosynthesis of alkaloids

#### CHEMCOR17: Physical Chemistry – 4 [Credits – 4]

#### **Unit-1: Quantum Mechanics and Spectroscopy**

Theoretical basis of interaction of radiation with matter: Harmonic perturbation and transition probabilities, Selection rule for vibrational spectra, anharmonic correction by perturbation - appearance of overtones, selection rule for rotational spectra, Raman scattering, Application of group theory to molecular vibrations, Normal modes, Vibrational transitions, IR and Raman Spectra and Selection rule

#### **Unit 2: Material Chemistry**

Conductors, Semi-conductors and Insulators; p-n junction semi-conductors (intrinsic and extrinsic), Theoretical basis: Free electron theory of metals, chemical and quantum mechanical concept, specific heat, Hall effect and its quantum manifestation, Band theory of metals: band gap, electrical and thermal conductivity of metals. Super conductors.

#### Unit-3: Laser and advanced Photophysics

Principles of Laser and Maser action. Population inversion (two/three/four level systems). Basic elements in Laser, Characteristics of Laser Radiation, CW and Pulsed Laser, Harmonic generation, Applications. Excited state inter and intra molecular proton transfer reactions, Excimer and Exciplex formation Excited state electron transfer processes, Marcus theory of electron transfer processes. Forster resonance energy transfer (FRET) and its applications

#### **Unit-4: Bio-physical Chemistry**

Configuration and conformation of biological macromolecules. Membrane structure. Spectroscopic methods: UV-Vis and CD. Separation techniques : Gel Electrophoresis. Macromolecule-ligand binding and cooperativity, Drug-DNA interaction.

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#### **CHEMDSE02:** Elective [Credits – 4]

#### **Inorganic Chemistry**

#### **Unit 1: Advanced bio-inorganic Chemistry**

Metal ions in genetic information transfer: Interactions of metal ions with purine and pyrimidine bases, nucleosides, nucleotides (especially ATP) and nucleic acids DNA and RNA.

Metal ions in metabolic energy transfer: Biological phosphate esters and their phosphate transfer potentials, mechanisms of non-enzymatic ATP hydrolysis (uncatalyzed, metal ion catalyzed and metal complex catalyzed) as models.

Bioinorganic chemistry of human iron metabolism: Ferritin, transferrin, siderophores (siderochromes) and ceruloplasmin.

Hydrolytic metalloenzymes: Active site structures and mechanism of actions of urease, carbonicanhydrases, carboxypeptidases.

Redox metalloenzymes: Active site structures and mechanism of actions of catalase, peroxidase, haloperoxidases, cytochrome *P*-450, nitric oxide synthases (NOS); super oxide dismutase (SOD), ascorbate oxidase; molybdoenzymes: aldehyde oxidase, sulfite oxidase, xanthine oxidase, nitrate reductases.

Vitamins and coenzymes: Vitamin B6 and vitamin B12 coenzymes, model systems

#### Unit 2: Spectroscopic analysis of inorganic compounds

Application of IR, UV, NMR, ESR, Mossbauer spectroscopy in inorganic chemistry (examples with simple and complex inorganic compounds including organometallic and cluster compounds and bio inorganic system).

Solid state reactions: Kinetics of solid state reactions by TGA, DTA and DSC methods (typical examples)

#### **Unit 3: Inorganic reaction mechanism**

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), and redox catalyzed substitution reactions.

Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Four broad classes of mechanism of substitution-D, A,  $I_a$  and  $I_d$ . Mechanism of isomerization reaction-linkage isomerism, cis- trans isomerism, intramolecular and intermolecular racemisation, Ray-Dutt and Bailartwist mechanisms.

#### **Unit 4: Crystallography**

Fundamentals of X-ray crystallography, crystal forms, lattice, primitive cell, crystal systems and symmetry, non-primitive lattices, crystal classes, space groups, crystals and their properties, Diffraction of x-ray, lattice planes, indices, Bragg's condition, reciprocal lattice, Bragg's law in reciprocal, Geometric data collection (simple examples), structure factor, systematic absence, heavy atom method. Fourier synthesis, Patterson function, experimental diffraction methods (Laue method, rotating crystal method).

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#### 13M

**12M** 

### Organic Chemistry

#### Unit 1: Advanced Stereochemistry

Advanced course involving conformation and reactivity, cyclic system, monocyclic systems- small and medium rings, 6-4, 5-5 bicyclic systems, 6-6-6, 6-5-6, 5-6-6, 5-5-5 tricyclic systems.

Chiroptical properties of organic molecules: origin, theory of CD, ORD principles and applications, Haloketone rule, Sector rule, Helicity rule.

#### **Unit 2: Advanced Pericyclic Reactions**

General perturbation molecular orbital theory in cycloaddition reaction: Reactivity, Regioselectivity and Periselectivity, correlation diagrams, 1,3-dipolar cycloaddition, Cycloadditions involving more than six electrons, Three and four component cycloaddotion, Ene reactions, Group transfer reactions and eliminations, Electrocyclic reactions of charged systems, Sigamatropic rearrangement: [1,5] and [1,7] shifts in neutral systems and [1,4] shift in charged species, [3,3] shifts, Cope rearrangements, Claisen rearrangement, [5,5] shifts, [2,3] shifts in ylides.

#### Unit 3: Advanced NMR spectroscopy

Application of DEPT,<sup>1</sup>H-<sup>1</sup>H COSY, HMBC, HMQC, TOCSY, NOESY in structure elucidation of organic compounds, drug screening, reaction monitoring etc., Solid state NMR (CP-MAS). Application of spectral data (IR, UV, <sup>1</sup>H-NMR, <sup>13</sup>C-NMR & Mass Spectrometry)

#### Unit 4: Molecules of Life

Proteins: Structure and function

Carbohydrates: Structure of di- and poly-saccharides

Nucleic acids: Chemical synthesis of nucleosides and oligonuleotides, Bio-synthesis of nucleotides and folic acids, Replication, transcription- Protein bio-synthesis, Covalent interaction of nucleic acids with small molecules, Structural features of DNA and RNA.

#### **Physical Chemistry**

#### **Unit-1: Advanced Quantum Mechanics**

Manyelectron systems: Closed and open shells, Antisymmetric principle and antisymmetrizer operator. Independent particle model (IPM). Self-consistent fields: Hartree and Hartree-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). Multidimensional wave function and configuration interaction. Brillouin's theorem. Application of ab initio methods, Density functional theory, Applications.Virial theorem and chemical bonding; Hellmann-Feynman theorem, Electrical responsive properties.

#### Unit 2 : Non-equilibrium thermodynamics

Meaning and scope of irreversible thermodynamics, Thermodynamic criteria for non-equilibrium states, balance equations for irreversible processes, Phenomenological equations, microscopic reversibility and Onsager reciprocity relations, examples and illustrations. , Entropy production- specific examples of entropy production, Non-equilibrium stationary states, Prigogine's principle of entropy production, Coupled phenomena, Some important applications.

#### 13M

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### 12M

# 13M

Unit-3: Macromolecules

Definition of Polymers; Types of Polymers; Polymerization process – condensation, addition, radical chain, ionic, condensation polymerization, copolymerization; Kinetics of Polymerization, chain transfer, retardation, inhibition; Polymerization in homogeneous and heterogeneous systems; Polymerization conditions; Mechanisms of polymerization; Molecular mass of Polymers, their determination. Biomacromolecules (Proteins & DNA).

#### **Unit-4 : Statistical Mechanics III**

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-Einstein condensation.

#### CHEMDSE03: Laboratory Experiment and Research Project [Credits – 8] 100M

Unit 1:

#### **Inorganic: Physico-chemical experiment**

1.Determination of composition of complexes formed in solution by spectrophotometric methods:

(a) Mole-ratio method

(b) Slope- ratio method

(c) Job's method of continuous variation

Model systems:(i) Fe(III)-sulfosalicylic acid complex(ii) Fe(II)-(1,10- phenanthroline) complex

(iii) Cu(II) - ethylenediamine complex

2. Determination of stability constants of metal-ligand complexes by pH-metric methods:

Model systems: (i) Cu(II)glycinate complexes(ii) Cu(II)-sulfosalicylate

3. Kinetic study on consecutive reactions:

Model system: Determination of the rates of consecutive aquation of the complex,

H[Co(III)(DMGH)<sub>2</sub>Cl<sub>2</sub>], by conductance method (where, DMGH= dimethylglyoximate monoanion).

4. Kinetics studies on redox reactions:

Model system: Determination of the rate constants of reduction of the complex,  $[Co(NH_3)_5(N_3)]Cl_2$  spectrophotometrically, by aqueous Fe(II) ion.

5. Kinetics studies on substitution reactions:

Model system: Kinetic investigation of the substitution reaction,  $[Co(NH_3)_5(SO_3)]^+ + NO_2^- \rightarrow by$  spectrophotometric method.

#### **Organic: Multistep organic synthesis**

Synthesis of model organic compounds involving typical multi step reactions, isolationand purification of the intermediate and the final products (as applicable) and their characterization by recrystallization, chromatographic separation (as applicable), determination of m.p / b.p (as the case may be), and spectral measurements.

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#### **Physical: Spectrophotometric experiment**

1. Determination of molecular weight of PVA by viscosity measurement.

2. Determination of the  $Fe^{2+}$  - orthophenanthroline complex by Job's continued variation method.

3. Spectrophotometric determination of Isosbestic point of Bromocresol Green indicator.

4. Kinetic Study of the Iodination of Aniline by Colorimetric Method.

5. Spectrophotometric study of the alkaline hydrolysis of Crystal Violet. (Determination of rate constant "k" and order "n" with respect to alkali)

#### Unit 2: Project work

During Semester-IV, each candidate shall carry out some investigative work independently or under the supervision of one or more guides(s), who may be Teacher / Guest Teacher / Member of P.G Board of Studies of the College / University / Scientist of any Recognized Research Institute. The work may be carried out either in the College / University itself or in any Recognized Research Institute, with the approval of the appropriate authority of the College/ University. Duration of the work shall be four weeks (approximately 90-100 hours). The findings of the project work should be submitted in the form of a dissertation for evaluation by an External Expert, not related in any way with the project work.

#### **Unit 3: Literature Review**

Each candidate shall present his /her project work and/or recent interesting published paper in a departmental seminar during a period not exceeding 20 minutes.

Unit 4: Grand Viva

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**30M**