SEMES-	CORE COURSE	ABILITY	SKILL	DISCIPLINE	`GENERIC
TER	(14)	ENHANCEMENT COMPULSORY	ENHANCEME	SPECIFIC ELECTIVE – DSE(4)	ELECTIVE COURSE –
		COURSE – AECC(2)	SEC(2)		GE(4)
(1)	(2)	(3)	(4)	(5)	(6)
	(Core/Chem/TH/01)	AECC – 1/2/			GE/Chem/TH/01
(I)	(Core/Chem/PR/01)	(Englísh)			GE/Chem/PR/01
					(6)
	(Core/Chem/TH/02)				
	(Core/Chem/PR/02)				
	(Core/Chem/TH/03)	AECC – 2/2/			GE – 2(6)
(II)	(Core/Chem/PR/03)	(ENV. SC.)			(Math.)
	(Core/Chem/TH/04)				
	(Core/Chem/PR/04)				
	(Core/Chem/TH/05)		SEC – 1(2)		GE – 3 <i>(6)</i>
(III)	(Core/Chem/PR/05)		Comp.		(Math.)
			C ⁺⁺ (Faculty)		
	(Core/Chem/TH/06)				
	(Core/Chem/PR/06)				
	(Core/Chem/TH/07)				
	(Core/Chem/PR/07)				
	(Core/Chem/TH/08)		SEC/Chem/02		GE/Chem/TH/04
(IV)	(Core/Chem/PR/08)				GE/Chem/PR/04
					(6)
	(Core/Chem/TH/09)				
	(Core/Chem/PR/09)				
	(Core/Chem/TH/10)				
	(Core/Chem/PR/10)				
	(Core/Chem/TH/11)			DSE/Chem/TH/01	
(V)	(Core/Chem/PR/11)			DSE/Chem/PR/01 (6)	
	(Core/Chem/TH/12)			DSE/Chem/TH/02	
	(Core/Chem/PR/12)			DSE/Chem/PR/02 (6)	
	(Core/Chem/TH/13)			DSE/Chem/TH/03	
(VI)	(Core/Chem/PR/13)			DSE/Chem/PR/03 (6)	
	(Core/Chem/TH/14)			DSE/Chem/TH/04	
	(Core/Chem/PR/14)			DSE/Chem/PR/04 (6)	
	(84)	(04)	(04)	24	24 = (140)

PROPOSED SCHEME FOR CHOICE BASED CREDIT SYSTEM IN B. Sc. Chemistry(Honours)

 $Col.No.-2: UG/Sc./Core/Phy., Chem., Math., Geog., Geol., /(TH/01 - 14) \ and \ (PR/01-14).$

Col.No.-3: UG/Sc./AECC/01, 02.

Col.No.-4: UG/Sc./SEC/01, 02.

Col.No.-5: UG/Sc/DSE/ 01 – 04.

Col.No.-6: UG/Sc./GE/01 – 04.

Chemistry (1	Tonors) Courses.							
Semester	Theoretical (1 Cr	edit $\equiv 1L/W$)	Practical (1 Cr	Total			
(~15 Weeks)	(1 L/W≡ 1 Lecture of 1 H	lour period/	Week)	(1 L/W≡ Laboratory Teac	atory Teaching of 1Hour / Week)			
		Credit	Full		Credit	Full Marks		
	No. of Papers	of each	Marks	No. of Papers	of each	of each		
		Paper			Paper	paper		
Ι	2	4	50	2	2	50	200	
II	2	4	50	2	2	50	200	
III	3	4	50	3	2	50	300	
IV	3	4	50	3	2	50	300	
V	4	4	50	4	2	50	400	
Core	<mark>14</mark>	<mark>56</mark>	<mark>700</mark>	14	<mark>28</mark>	<mark>700</mark>	<mark>1400</mark>	
Course	(Core/Chem/TH/01-14)			(Core/Chem/PR/01-14)				
Total								
Ι	1(AECC-1)	2	50	1			50	
	(English)							
II	1(AECC-2)	2	50	1			50	
	(Env. Sc.)							
III	1(SEC-1)	2	50	1			50	
	(Computer C++)							
IV	1(SEC-2)	2	50	1			50	
	(SEC/Chem/02)							
VI	4	4	50	4	2	50	400	
	(DSE/Chem/TH/01-04)			(DSE/Chem/PR/01-04)				
Non-Core	8	<mark>24</mark>	<mark>400</mark>	<mark>4</mark>	<mark>8</mark>	200	<mark>600</mark>	
Total								
Total	22	80		18	36		2000	

Jadavpur University B. Sc. Course Structure of 3 Year (6 Semester)

GE(General Elective) Courses :

Ι	1(GE/Chem/TH//01)	4	50	1(GE/Chem/PR/01)	2	50	100
II	1(GE/Math/TH/02)	5		1(GE/Math/TU/02)	1		100
III	1(<mark>GE/Math/TH/03</mark>)	5		1(<mark>GE/Math/TU/03</mark>)	1		100
IV	1(<mark>GE/Chem/TH/0</mark> 4)	4	50	1(GE/Chem/PR/04)	2	50	100
GE-Total	<mark>4</mark>	<mark>18</mark>		<mark>4</mark>	<mark>6</mark>		<mark>400</mark>
Grand	26 (Theory Papers)	98		22(Lab/Tutorial Papers)	42		2400
Total							
(140							
Credit)							

Abbreviations:

Chem : Chemistry; TH: Theory; PR: Practical; AECC: Ability Enhancement Compulsory Course; SEC: Skill Enhancement Course; DSE: Discipline Specific Elective; GE: Generic Elective;; TU: Tutorial; I: Inorganic; O: Organic; P: Physical; L: Laboratory;

Unit Nomenclature:

Illustration: 4031-P

[1st Digit (4): Semester No.; 2nd & 3rd Digits (03): Paper No.; 4th Digit (1): Unit No.; Last Letter (P): Physical Chemistry]

An Overview of B. Sc. Chemistry (Honors) with Course Content Keywords

Abbreviations:

TH: Theory; PR: Practical; L: Laboratory; I: Inorganic; O: Organic; P: Physical; SEC: Skill Enhancement Course; DSE: Discipline Specific Elective

	Theo	Paper	Unit No.	Content Keywords	Lecture	Marks	Credit
Sem	/Lab	(Marks)		, ,	s		
No.	(Full				/ Week		
	Marks)				(L/W)		
I (200)	TH (100)	Chem/TH/01 (50)	1011-I	Extra Nuclear Structure of Atom; Periodicity of Elements	2	25	2
			1012-P	Unit & Dimension; Gaseous State (Ideal & Real): Intermolecular Forces	2	25	2
		Chem/TH/02 (50)	1021-O	Organic Chemistry I: Basics of Organic Chemistry	2	25	2
		()	1022-O	Stereochemistry-I	2	25	2
	PR	Chem/PR/01	101L-O	Organic Chemistry-I	4	50	2
	(100)	Chem/PR/02	102L-P	Physical Chemistry-I	4	50	2
II	TH	Chem/TH/03	2031-I	Bonding – I; Radioactivity	2	25	2
(200)	(100)	(50)	2032-О	Organic Chemistry II	2	25	2
		Chem/TH/04	2041-P	Thermodynamics-I; Liquid State	2	25	2
		(50)	2042-P	Chemical Kinetics & Catalysis	2	25	2
	PR	Chem/PR/03	203L-I	Inorganic Chemistry-I	4	50	2
	(100)	Chem/PR/04	204L-O	Organic Chemistry-II	4	50	2
III	TH	Chem/TH/05	3051-I	Redox: Acid-Base and Non-aqueous	2	25	2
(350)	(150)	(50)		solvents	_		_
			3052-I	Bonding–II; Comparative study of Group elements–I (s–block elements; noble gases)	2	25	2
		Chem/TH/06	3061-O	Chemistry of alkenes and alkynes;	2	25	2
		(50)		Aromatic Substitution; Organometallics and conjugate additions			
			3062-O	Carbonyl and Related Compounds.	2	25	2
		Chem/TH/07 (50)	3071-P	Thermodynamics-II & Chemical	2	25	2
		(00)	3072-P	Quantum Mechanics-I: Solid State	2	25	2
	TH+Tu	SEC/01		(To be offered by Science Faculty (SEC-1))	4	50	2
	(50)	520,01			·	00	-
	PR	Chem/PR/05	305L-I	Inorganic Chemistry-II	4	50	2
	(150)	Chem/PR/06	306L-P	Physical Chemistry-II	4	50	2
		Chem/PR/07	307L-P	Physical Chemistry-III	4	50	2
IV (350)	TH (150)	Chem/TH/08 (50)	4081-I	Coordination Chemistry–I; Molecular symmetry and Point Groups	2	25	2
()	()	()	4082-I	Chemistry of p- Block Elements	2	25	2
		Chem/TH/09	4091-O	Nitrogen compounds: Rearrangements:	2	25	2
		(50)	4092-O	The Logic of Organic Synthesis; Organic	2	25	2
		Chem/TH/10	4101-P	Colligative Properties & Phase Equilibria	2	25	2
		(50)	4102-P	Transport Properties & Conductance	2	25	2
		(00)	11021	Photochemistry-I	-		
	TH	SEC/Chem/TH/02	SEC02-I	Errors in Chemical Analysis; Use of organic	2	50	2
	SEC/02/	(50)		reagents; Analysis of Soil. Analysis of			
	(50)			water, Food Products, Cosmetics & Other			
	DD	Cl /DD /00	4001 1	Applications		50	2
	PK (150)	Chem/PR/08	408L-1	Inorganic Chemistry-III	4	50	2
	(150)	Chem/DD/10	409L-0	Organic Chemistry IV	4	50	2
1	I		1 +10L-O	Organic Chemistry-1v	4	50	L 2

V	TH	Chem/TH/11	5111-I	Coordination Chemistry-II; Colour,	2	25	2
(400)	(200)	(50)		Magnetism and Bioinorganic Chemistry			
			5112-I	Transition Elements and Lantha-noids and Actinoids	2	25	2
		Chem/TH/12 (50)	5121-0	Carbocycles, Heterocycles and Cyclic stereochemistry	2	25	2
		((**))	5122-0	Pericyclic reactions and Biomolecules.	2	25	2
		Chem/TH/13	5131-P	Adsorption & Colloids; Nanomaterials;	2	25	2
		(50)		Polymer			
			5132-P	Electrochemistry-II	2	25	2
		Chem/TH/14 (50)	5141-I	Organometallics; Inorganic Reaction Mechanism and Coordination Chemistry of Non-transitional elements.	2	25	2
			5142-P	Quantum Mechanics-II; Electrical &	2	25	2
				Magnetic Properties of Materials			
	PR	Chem/PR/11	511L-I	Inorganic Chemistry-IV	8	100	4
	(200)	Chem/PR/12	512L-I				
		Chem/PR/13	513L-O	Organic Chemistry-V	4	50	2
		Chem/PR/14	514L-P	Physical Chemistry-IV	4	50	2
VI	TH	DSE/Chem/TH/01	6011-I	Analytical Methods in Chemistry – I :	2	25	2
(400)	(200)	(50)		Optical methods of analysis; Thermal and			
		(Any one unit to be		Electro analytical methods of analysis			
		chosen)		Analytical Methods in Chemistry – II :	2	25	2
				Separation Techniques			
			6012-I	Instrumental Methods of Chemical Analysis	4	50	4
		DSE/Chem/TH/02	6021-O	Green Chemistry - I	2	25	2
		(50)	6022-O	Green Chemistry - II	2	25	2
		DSE/Chem/TH/03	6031-P	Photo chemistry-II & Spectroscopy	2	25	2
		(50)	6032-P	Statistical Thermodynamics	2	25	2
		DSE/Chem/TH/04	6041-I	Industrial Chemistry	2	25	2
		(50)		Environmental Chemistry	2	25	2
		(Any one unit to be	6042-O	Polymer Chemistry	4	50	4
		chosen)	6043-P	Application of Computers in Chemistry	4	50	4
	PR	DSE/Chem/PR/01	6011L-I	Inorganic Chemistry-V	4	50	2
	(200)	(One unit as in	6012L-I	Instrumental Methods of Chemical Analysis	4	50	2
		DSE/Chem/TH/01)					
		DSE/Chem/PR/02	602L-O	Organic Chemistry-VI	4	50	2
		DSE/Chem/PR/03	603L-P	Physical Chemistry-V	4	50	2
		DSE/Chem/PR/04	604L-I	Project-Seminar/Review	4	50	2
		(I/O/P to be chosen	604L-O	Project-Seminar/Review	4	50	2
		as in DSE/Chem/TH/04)	604L-P	Application of Computers in Chemistry	4	50	2

An Overview of GE Courses Offered in Chemistry along with the Course Content Keywords

Sem No.	Theo /Lab	Paper (Marks)	Unit No.	Unit title	Periods / Week	Marks	Credit
I (100)	TH (50)	GE/Chem/TH//01	101G-I	Inorganic Chemistry-I Inorganic Chemistry-II	2	25	2
			101G-O	Organic Chemistry -I	2	25	2
	PR (50)	GE/Chem/PR//01	101G-L	Inorganic Chemistry Experiments	4	50	2
II (100)	TH+TU	GE/Math/TH/02		(To be offered by Mathematics Dept.)		100	6
III (100)	TH+TU	GE/Math/TH/03		(To be offered by Mathematics Dept.)		100	6
IV	TH (50)	GE/Chem/TH/04	404G1-P	Physical Chemistry-I	2	25	2
(100)			404G2-O 404G2-P	Organic Chemistry-II Physical Chemistry-II	2	25	2
	PR (50)	GE/Chem/PR/04	404G-L	Organic & Physical Chemistry Experiments	4	50	2
				Total		400	24

Jadavpur University B. Sc. Chemistry (Honours) 3 Year (6 Semester) Syllabus

Semester –I

Theory Papers:

Paper: Chem/TH/01: (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit: 1011-I :</u> Extra Nuclear Structure of Atom; Periodicity of Elements (30L)

A. Extra Nuclear Structure of Atom [15 L]:

Bohr's theory, its limitations and atomic spectrum of hydrogen atom, Sommerfeld's Theory, Wave mechanics, de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2 , Quantum numbers and their significance, Zeemann effect, Normalized and orthogonal wave functions, Sign of wave functions, Radial and angular wave functions for hydrogen atom, Radial and angular distribution curves, Shapes of *s*, *p*, *d* and *f* orbitals, Contour boundary and probability diagrams.

Pauli's Exclusion Principle, Hund's rules, Exchange energy, Aufbau principle and its limitations, Ground state Term symbols of atoms and ions for atomic number up to 30, Excited State Term Symbol (e.g., 2s¹2p¹, 3p¹3d¹etc)

B. Periodicity of Elements (15 L):

Modern IUPAC Periodic table, Effective nuclear charge, screening effects and penetration, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii and crystal radii. Scandide contraction, lanthanide contraction. Ionization enthalpy, successive ionization enthalpies and factors affecting ionization energy and the application of ionization enthalpies. Electron affinity and Electronegativity (Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffé's electronegativity scales). Variations of electronegativity with bond order, partial charge, hybridization. Group electronegativities. Sanderson's electron density ratio. Group trends and periodic trends in these properties in respect of s-, p-, d- and f-block and elements. Secondary periodicity, Relativistic Effect, Inert pair effect.

<u>Unit: 1011-P</u> :Unit & Dimension; Gaseous State (Ideal & Real gases); Intermolecular forces (30L)

Unit & Dimension (5 L)

Physical quantities, definition, dimensions & units (emphasis on SI units).

Gaseous State: Ideal gases (12 L)

Recapitulation of gas laws, postulates of Kinetic theory, distribution of velocity, speed, and translational kinetic energy, Kinetic gas equation (expression for gas pressure), root mean square (rms) speed, average translational kinetic energy (KE), absolute scale of temperature, Barometric distribution law.

Maxwell-Boltzmann distribution law of molecular velocities, speed and translational kinetic energy in one-, two-, three dimensions, calculation of most probable, average and rms values in each case, independent mode of motion or degree of freedom, principle of equipartition of energy, molecular basis of heat capacity, deviation, bimolecular collision, collision cross section, collision frequencies (similar & dissimilar molecules), wall collision frequency & rate of diffusion, mean free path.

Real gases (10 L)

Coefficient of expansion & compression, deviation from ideality, compressibility factor, Andrew's & Amagat's experiments, van der Waals equation of state and its critical constants, Boyle temperature, reduced equation of state, Law of corresponding states, other equations of state, virial equation of state.

Intermolecular forces (3 L)

Dipole-dipole (Keesom), dipole-induced dipole (Debye) & induced dipole-induced dipole (London) interactions; model interaction potentials (hard sphere, square well, Sutherland and LJ potential); liquefaction of gases.

Paper: Chem/TH/02 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 1021-O</u> : Basics of Organic Chemistry (30L)

A. Bonding and Physical Properties:

- 1. Valence Bond Theory: Concept of hybridisation, shapes of molecules, resonance (including hyperconjugation); calculation of formal charges and double bond equivalent (DBE); orbital pictures of bonding (sp³, sp², sp: C-C, C-N & C-O systems and *s*-cis and *s*-trans geometry for suitable cases).
- 2. Electronic displacements: Inductive effect, field effect, mesomeric effect, resonance energy, bond polarization and bond polarizability, electromeric effect, steric effect, steric inhibition of resonance.
- **3. Physical properties:** Influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle strain (Baeyer's strain theory); melting point/boiling point and solubility of common organic compounds in terms of covalent & non-covalent intermolecular forces; polarity of molecules and dipole moments; relative stabilities of isomeric hydrocarbons in terms of heat of hydrogenation, heat of combustion and heat of formation.
- 4. **Reaction thermodynamics:** Free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change via BDE, intermolecular & intramolecular reactions.
- 5. MO theory: Qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about σ , σ^* , π , π^* , n-MOs; basic idea about Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; interpretation of chemical reactivity in terms of FMO interactions; sketch and energy levels of π MOs of i) acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems), ii) cyclic p orbital system (neutral systems: [4], [6]-annulenes; charged systems: 3-, 4-, 5-membered ring systems); Hückel's rules for aromaticity up to [10]-annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram; elementary idea about α and β ; measurement of delocalization energies in terms of β for buta-1,3-diene, cyclobutadiene, hexa-1,3,5-triene and benzene.

B. General Treatment of Reaction Mechanism-I:

- 1. Mechanistic classification: Ionic, radical and pericyclic (definition and example); reaction type: addition, elimination and substitution reactions (definition and example); nature of bond cleavage and bond formation: homolytic and heterolytic bond fission, homogenic and heterogenic bond formation; curly arrow rules in representation of mechanistic steps; reagent type: electrophiles and nucleophiles (elementary idea); electrophilicity and nucleophilicity in terms of FMO approach.
- 2. Reactive intermediates: Carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes: generation and stability, structure using orbital picture and electrophilic/nucleophilic behavior of reactive intermediates (elementary idea).

Unit : 1022-O : Stereochemistry-I (30L)

- 1. Bonding geometries of carbon compounds and representation of molecules: Tetrahedral nature of carbon and concept of asymmetry; Fischer, sawhorse, flying-wedge and Newman projection formulae and their inter translations.
- 2. Relative and absolute configuration: D/L and R/S descriptors; erythro/threo and meso nomenclature of compounds; syn/anti nomenclatures for aldols; E/Z descriptors for C=C, conjugated diene, triene, C=N and N=N systems; combination of R/S- and E/Z- isomerisms.
- **3. Optical activity of chiral compounds:** optical rotation, specific rotation and molar rotation; racemic compounds, racemisation (through cationic, anionic, radical intermediates and through reversible formation of stable achiral intermediates).
- 4. Concept of chirality and symmetry: Symmetry elements, molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of epimers; concept of stereogenicity, chirotopicity and pseudoasymmetry; chiral centres and number of stereoisomerism: systems involving 1/2/3-chiral centre(s) (AA, AB, ABA and ABC types).

5. Conformation: Conformational nomenclature: eclipsed, staggered, gauche, syn and anti; dihedral angle, torsion angle; Klyne-Prelog terminology; P/M descriptors, energy barrier of rotation, concept of torsional and steric strains; relative stability of conformers on the basis of steric effect, dipole-dipole interaction and H-bonding; butane gauche interaction; conformational analysis of ethane, propane, n-butane, 2-methylbutane and 2,3-dimethylbutane; haloalkane, 1,2-dihaloalkanes and 1,2-diols (up to four carbons); 1,2-halohydrin; conformation of conjugated systems (*s*-cis and *s*-trans).

Laboratory experiments:

Paper : Chem/PR/01: (2 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 101L-O</u>: Organic Chemistry-I Basics of Organic Chemistry

1. Separation: Based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO₃, etc., of components of a binary solid mixture; purification of any one of the separated components by crystallization and determination of its melting point. The composition of the mixture may be of the following types: Benzoic acid/p-Toluidine; p-Nitrobenzoic acid/p-Aminobenzoic acid; p-Nitrotolune/p-Anisidine; etc.

2. Determination of boiling point: Determination of boiling point of common organic liquid compounds e.g., ethanol, cyclohexane, chloroform, ethyl methyl ketone, cyclohexanone, acetylacetone, anisole, crotonaldehyde, mesityl oxide, etc. [Boiling point of the chosen organic compounds should preferably be less than 160 °C]

3. Identification of a pure organic compound: Solid compounds: oxalic acid, tartaric acid, citric acid, succinic acid, resorcinol, urea, glucose, cane sugar, benzoic acid and salicylic acid; Liquid Compounds: formic acid, acetic acid, methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene.

Paper : Chem/PR/02 : (2 Credit, FM-50, 4 L/W; 60L)

Unit : 102L-P : Physical Chemistry-I

List of Experiments:

- 1. Instruction for students on primary & secondary standard solution and its preparation, weighing, pipetting, titration, cleaning & handling of apparatus, related things.
- 2. Determination of the strength of supplied acid solution.
- 3. Determination of the strength of supplied thiosulphate solution iodometrically.
- 4. Determination of the surface tension of supplied solutions by drop weighing method.
- 5. Determination of the viscosity coefficient of supplied liquid using Ostwald Viscometer.
- 6. Determination of the distribution coefficient of iodine between non aqueous and aqueous solvents.
- 7. Determination of pH of a solution by colour matching method.

Semester -II

Theory Papers:

Paper: Chem/TH/03: (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 2031-I</u> : Bonding- I; Radioactivity (30L)

A. Bonding – I (15 L):

General characteristics, types of ions, size effects, radius ratio rule and its application and limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. The Born-Mayer equations; Madelung constant, Born-Haber cycle and its application, Solvation energy. Illustration of Wurtzite, Rutile, Anti-rutile, Fluorite, Anti-Fluorite, Perovskite, Antiperovskite etc. structures with suitable examples.

Covalent bond: Polarizing power and polarizability, ionic potential, Fazan's rules. Lewis structures, Resonance of inorganic ions & formal charge. Valence Bond Theory. The hydrogen molecule (Heitler-London approach), directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals, Dipole moments, VSEPR theory, shapes of molecules and ions containing lone pairs and bond pairs (examples from main groups chemistry) and multiple bonding (σ and π bond approach), stereochemically inactive lone pair, Bent's rule and its theoretical basis, Berry Pseudo rotation.

B. Radioactivity (15 L):

- 1. Disintegration Laws and Radioactive equilibrium.
- 2. Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (Liquid Drop and Shell Model): Concept of nuclear quantum number, magic numbers.
- 3. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes.
- 4. Chemical effects of nuclear transformation–Szillard–chalmer effect, recoil energy, effects due to isomeric transitions, also nuclear spin effect leading to ortho–and para–forms of H₂, N₂, F₂ molecules.
- 5. Radio chemical methods: principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures.

<u>Unit : 2032-O</u> : Organic Chemistry-II (30L)

A. Stereochemistry–II (7 L):

- 1. Chirality arising out of stereoaxis: Stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkylidene cycloalkanes and biphenyls; related configurational descriptors (aR/aS and P/M); atropisomerism; racemisation of chiral biphenyls; buttressing effect.
- 2. Concept of prostereoisomerism: Prostereogenic centre; concept of (pro)n-chirality: topicity of ligands and faces (elementary idea); pro-R/pro-S, pro-E/pro-Z and Re/Si descriptors; pro-r and pro-s descriptors of ligands on pro-pseudoasymmetric centre.

B. General Treatment of Reaction Mechanism-II (8 L):

- 1. **Reaction kinetics:** Rate constant and free energy of activation; concept of order and molecularity; free energy profiles for one-step, two-step and three-step reactions; catalyzed reactions: electrophilic and nucleophilic catalysis; kinetic control and thermodynamic control of reactions; isotope effect: primary and secondary kinetic isotopic effect (k_H /k_D); principle of microscopic reversibility; Hammond's postulate.
- 2. Tautomerism: Prototropy (keto-enol, nitro aci-nitro, nitroso-oximino, diazo-amino and enamine-imine systems); valence tautomerism and ring-chain tautomerism; composition of the equilibrium in different systems (simple carbonyl; 1,2- and 1,3-dicarbonyl systems, phenols and related systems), factors affecting keto-enol tautomerism; application of thermodynamic principles in tautomeric equilibria.
- **3.** Concept of organic acids and bases: Effect of structure, substituent and solvent on acidity and basicity; proton sponge; gas-phase acidity and basicity; comparison between nucleophlicity and basicity; HSAB principle; application of thermodynamic principles in acid-base equilibria.

C. Substitution and Elimination Reactions (15 L):

- 1. Free-radical substitution reaction: Halogentaion of alkanes, mechanism (with evidence) and stereochemical features; reactivity-selectivity principle in the light of Hammond's postulate.
- 2. Nucleophilic substitution reactions: Substitution at sp³ centre: mechanisms (with evidence), relative rates & stereochemical features: S_N1, S_N2, S_N2', S_N1' (allylic rearrangement) and S_Ni; effects of solvent, substrate structure, leaving group and nucleophiles (including ambident nucleophiles, cyanide & nitrite); substitutions involving NGP; role of crown ethers and phase transfer catalysts; [systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides].
- **3.** Elimination reactions: E1, E2, E1cB and Ei (pyrolytic *syn*-eliminations); formation of alkenes and alkynes; mechanisms (with evidence), reactivity, regioselectivity (Saytzeff/Hofmann) and stereoselectivity; comparison between substitution and elimination; importance of Bredt's rule relating to the formation of C=C.

Paper: Chem/TH/04: (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 2041-P</u> : Thermodynamics-I (20L); Liquid State (10L):

Thermodynamics-I (20 L):

Basic concepts, Zeroth and First Law:

Mathematical background, thermodynamic terms, intensive & extensive variables, isolated, closed and open systems, thermodynamic processes, cyclic processes, reversible and irreversible processes, IUPAC convention, thermodynamic functions (state & path) and their differentials (perfect & imperfect), Zeroth law of thermodynamics, concept of heat, work & temperature.

First law of thermodynamics, Internal energy (U), Enthalpy (H), relation between C_p and C_v . Calculation of W, Q, $\Delta U \& \Delta H$ for expansion of ideal and van der Waals gases under isothermal and adiabatic conditions for reversible and irreversible processes including free expansion, Joule's law, Joule-Thomson experiment, its coefficient and inversion temperature.

Thermochemistry:

Application of first law of thermodynamics, Laws of thermochemistry, standard state, enthalpy of formation, combustion, solution, dilution (including enthalpy of infinite dilution), neutralization, enthalpy of ionization and formation of ions, bond dissociation energy (calculation from thermochemical data), Born-Haber cycle for calculation of lattice energy, Kirchoff's equation, relation between ΔH and ΔU of a reaction.

Liquid State (10 L):

Qualitative treatment of the structure of the liquid state, physical properties of liquids including their methods of determination, vapour pressure, boiling point, freezing point, surface tension, viscosity, refractive index; Liquid crystals (elementary discussion on classification, structure and properties), preliminary idea regarding water structure.

<u>Unit : 2042-P</u> : Chemical Kinetics & Catalysis (30L):

Chemical Kinetics :

Concept of advancement of reaction, rate, order, rate constant/ coefficient, molecularity, differential & integrated rate equations of different order reactions, experimental methods for determination of order & rate constant of reaction;

Elementary reaction, law of mass action, multistep reactions, rate determining step, steady state approximation and derivation of rate equation, temperature dependence of reaction rates and Arrhenius equation, energy of activation, Arrhenius factor, differential & integrated rate equations of opposing, parallel & consecutive reactions, chain reactions;

Theories of reaction rates, collision theory, Lindemann theory of unimolecular reactions, transition state theory (elementary idea).

Catalysis :

Catalysis, homogeneous catalysis, acid-base catalysis, enzyme catalysis: Michaelis-Menten equation, Lineweaver-Burk plot, turnover number, elementary idea of inhibition, primary kinetic salt effect, and solvent effect (qualitative aspect) of solution phase reactions; auto catalysis: periodic reaction.

Laboratory experiments

Paper : Chem/PR/03: (2 Credit, FM-50, 4 L/W; 60L)

Unit : 203L-I : Inorganic Chemistry-II

Acid and Base Titrations

- 1. Estimation of carbonate and hydroxide present together in mixture.
- 2. Estimation of carbonate and bicarbonate present together in a mixture.
- 3. Estimation of free alkali present in different soaps/detergents.

Oxidation-Reduction Titrimetric

A. Titration with KMnO₄

- 1. Standardization of KMnO₄ solution with standard oxalic acid solution.
- 2. Estimation of Fe(II) using standardized KMnO₄ solution.

B. Titration with K₂Cr₂O₇

- 1. Estimation of Fe(II) using K₂Cr₂O₇ solution.
- 2. Estimation of Fe(III) using K₂Cr₂O₇ solution.
- 3. Estimation of Fe(II) and Fe(III) in a given mixture using K₂Cr₂O₇ solution.

Paper : Chem/PR/04 : (2 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 204L-O:</u> Organic Chemistry-II : Organic Preparations

- A. The following reactions are to be performed, noting the yield of the crude product:
 - 1. Nitration of aromatic compounds
 - 2. Condensation reactions
 - 3. Hydrolysis of amides/imides/esters
 - 4. Acetylation of phenols/aromatic amines
 - 5. Benzoylation of phenols/aromatic amines
 - 6. Side chain oxidation of aromatic compounds
 - 7. Diazo coupling reactions of aromatic amines
 - 8. Bromination of anilides using green approach (Bromate-Bromide method)
 - 9. Selective reduction of m-dinitrobenzene to m-nitroaniline

(Students must also calculate percentage yield, based upon isolated yield (crude) and theoretical yield.)

- **B.** Purification of the crude product is to be made by crystallisation from water/alcohol, crystallization after charcoal treatment, or sublimation, whichever is applicable.
- C. Melting point of the purified product is to be noted.

Semester -III

Theory Papers:

Paper: Chem/TH/05 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 3051-I</u> : Redox; Acid-Base and Non-aqueous solvents (30L):

A. Redox (15 L)

Elementary idea on standard redox potentials with sign conventions, Nernst equation (without derivation). Formal Potential, Influence of complex formation, precipitation and change of pH on redox potentials. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators. Redox potential diagram (Latimer and Frost diagrams) of common elements and their applications. Pourbaix diagram and discussion. Disproportionation and comproportionation reactions (typical examples).

B. Acid-Base and Non-aqueous solvents (15 L)

Acid-Base : Bronsted-Lowry's concept, relative strength of acids, Pauling's rules, Lux-Flood concept, Lewis concept, group characteristics of Lewis acids, solvent leveling and differentiating effects. Thermodynamic acidity parameters, Drago-Wayland equation. Superacids, Gas phase acidity and proton affinity; HSAB principle, Pearson-Pauling paradox, Metal Aqua Complexes $[M(H_2O)_n]^{z+}$. Acid-base equilibrium in aqueous solution (Proton transfer equilibria in water), pH, buffer, Henderson equation. Common Ion effect and its applications in qualitative group analysis.

Non-aqueous Solvents: Physical properties of a solvent for functioning as an effective reaction medium - Types of solvents and their general characteristics - Reactions in liquid ammonia, liquid hydrogen fluoride and liquid sulphur dioxide.

<u>Unit : 3052-I</u> : Bonding-II; Comparative study of Group elements – I (s-block elements and noble gases) (30L):

A. Bonding –II (15 L):

Molecular orbital concept of bonding, Linear combination of atomic orbitals (LCAO) (elementary pictorial approach): sigma and pi-bonds and delta interaction, multiple bonding. Orbital designations, HOMO, LUMO. Orbital mixing, MO diagrams of H₂, Li₂, Be₂, B₂, C₂, N₂, O₂, F₂, and their ions wherever possible; Heteronuclear molecular orbitals: CO, NO, NO⁺, CN⁻, HF. Simple 3c-2e (H₃⁺) 3c-4e (H₃⁻), HF₂⁻, BeH₂. Bond properties: bond orders, bond lengths.

Weak Chemical Forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Intermolecular forces: Hydrogen bonding (theories of hydrogen bonding), receptor-guest interactions, Halogen bonds. Effects of chemical force, melting and boiling points etc.

B. Comparative study of Group elements-I (the s-block elements and the noble gases) (15 L):

The s-block elements of Gr – I, Gr – II, their general electronic configuration, trends in I. P., ionic radii;

- i) General metallurgical consideration of these elements.
- ii) Differences of Li and Be from other members of their groups (the diagonal relationship).
- iii) Comparative studies of Hydrides, Nitrides, Carbides and Oxides of Gr I, Gr II.
- iv) Compounds of Gr I, Gr II ions with Crown ether and Cryptands, Alkalides and Electride, Reverse sodium hydride.
- v) Isotopes of H, industrial preparation of deuterium, its properties, reactions and uses; ortho-para hydrogen.
- **C.** Nobel Gases: Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation, properties and reactivities of fluorides (XeF_n) and oxofluorides (XeO_mF_n) of xenon. Xenon-oxygen compounds. Molecular shapes of noble gas compounds. Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF₂ and XeF₄). Xenon-oxygen compounds. Fluorides of Krypton.

Paper: Chem/TH/06: (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 3061-O:</u> Chemistry of alkenes and alkynes; Aromatic Substitution; Organometallics and conjugate additions (30L):

A. Chemistry of alkenes and alkynes (10L) :

- 1. Addition to C=C: Mechanism (with evidence wherever applicable), reactivity, regioselectivity (Markownikoff and anti-Markownikoff additions) and stereoselectivity; reactions: hydrogenation, halogenations, iodolactonisation, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, epoxidation, syn and anti-hydroxylation, ozonolysis, addition of singlet and triplet carbenes; electrophilic addition to diene (conjugated dienes and allene); radical addition: HBr addition; mechanism of allylic and benzylic bromination in competition with brominations across C=C; use of NBS; Birch reduction of benzenoid aromatics; interconversion of *E* and *Z* alkenes; contra-thermodynamic isomerization of internal alkenes.
- Addition to C=C (in comparison to C=C): Mechanism, reactivity, regioselectivity (Markownikoff and anti-Markownikoff addition) and stereoselectivity; reactions: hydrogenation, halogenations, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, dissolving metal reduction of alkynes (Birch); reactions of terminal alkynes by exploring its acidity; interconversion of terminal and non-terminal alkynes.

B. Aromatic Substitution (10 L):

- 1. Electrophilic aromatic substitution: Mechanisms and evidences in favour of it; orientation and reactivity; reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction; one-carbon electrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Houben-Hoesch, Vilsmeier-Haack, Reimer-Tiemann, Kolbe-Schmidt); *ipso*-substituion.
- 2. Nucleophilic aromatic substitution: Addition-elimination mechanism and evidences in favour of it; S_NAr mechanism; cine substitution (benzyne mechanism), structure of benzyne.

C. Organometallics and conjugate additions (10 L):

- 1. Organometallics: Grignard reagents; Organolithiums; Gilman cuprates: preparation and reactions (mechanism with evidence); addition of Grignard and organolithium to carbonyl compounds; substitution on -COX; directed *ortho*-metalation of arenes using organolithiums, Shapiro reaction, conjugate addition by Gilman cuprates; Corey-House synthesis; abnormal behavior of Grignard reagents; comparison of reactivity among Grignard, organolithiums and organocopper reagents; Reformatsky reaction; Blaise reaction; concept of umpolung and base-nucleophile dichotomy in case of organometallic reagents.
- 2. Nucleophilic addition to α,β -unsaturated carbonyl system: General principle and mechanism (with evidence); direct and conjugate addition, addition of enolates (Michael reaction), Stetter reaction, Robinson annulations, Morita-Baylis-Hillman Reaction.

<u>Unit : 3062-O</u> :

Carbonyl and Related Compounds (30L):

- 1. Addition to C=O: Structure, reactivity and preparation of carbonyl compounds; mechanism (with evidence), reactivity, equilibrium and kinetic control; Burgi-Dunitz trajectory in nucleophilic additions; formation of hydrates, cyanohydrins and bisulphite adduct; nucleophilic addition-elimination reactions with alcohols, thiols and nitrogen- based nucleophiles; reactions: benzoin condensation, Cannizzaro and Tischenko reactions, reactions with ylides: Wittig and Corey-Chaykovsky reaction; McMuury reaction, Rupe rearrangement, Clemmensen, Wolff-Kishner, LiAlH₄, NaBH₄, MPV, Oppenauer, Bouveault-Blanc, acyloin condensation.
- 2. Exploitation of acidity of a-H of C=O: Formation of enols and enolates; kinetic and thermodynamic enolates; reactions (mechanism with evidence): halogenation of carbonyl compounds under acidic and basic conditions, Hell-Volhard-Zelinsky (H.V.Z.) reaction, nitrosation, condensations (mechanism with evidence): Aldol, Henry, Tollens', Knoevenagel, Claisen-Schmidt, Claisen ester including Dieckmann, Stobbe; Mannich reaction, Perkin reaction, Favorskii rearrangement; alkylation of active methylene compounds; preparation and synthetic applications of diethyl malonate and ethyl acetoacetate; specific enol equivalents (lithium enolates, enamines, aza-enolates and silylenol ethers) in connection with alkylation, acylation and aldol type reaction.
- **3.** Oxidizing agents: Oxidation of alcohols, aldehydes and ketones: chromium and manganese based reagents, Jones reagent, PDC, PCC and Swern oxidation; periodic acid, Dess Martin oxidation and lead tetraacetate oxidation of 1,2-diols and use of SeO₂ oxidation (Riley).
- 4. Substitution at sp² carbon (C=O system): Mechanism (with evidence): BAC2, AAC2, AAC1, AAL1 (in connection to acid and ester); acid derivatives: amides, anhydrides & acyl halides (formation and hydrolysis including comparison).

Paper: Chem/TH/07 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 3071-P</u> : Thermodynamics-II and Chemical Equilibrium (30 L)

Thermodynamics-II:

Engine, Heat engine, Carnot Engine and its efficiency, Refrigerator & Heat pump and their coefficient of performance, Kelvin-Planck & Clausius statement of second law, thermodynamic scale of temperature and concept of entropy, calculation of entropy changes for different processes, molecular interpretation of entropy, Gibbs free energy (G) & Helmholtz / work function (A) and their significances, thermodynamic criteria for equilibrium state and spontaneity, Maxwell relations, thermodynamic equations of state.

Nernst heat theorem, third law of thermodynamics, unattainability of zero Kelvin temperature adiabatic demagnetization.

Chemical Equilibrium:

Equilibria between different phases, phase transitions, order of phase transitions, Clapeyron equation, Clausius-Clapeyron equation, Trouton's Rule, open system: partial molar properties, chemical potential, Gibbs-Duhem equations, Chemical equilibria in homogeneous and heterogeneous systems, van't Hoff reaction isotherm, expression of equilibrium constants (K_c , K_p and K_x), pressure, temperature and concentration dependence of equilibrium constants, van't Hoff equation, Le Chatelier's principle & its thermodynamic support.

<u>Unit : 3072-P</u> : Quantum Mechanics-I; Solid state (30L) :

Quantum Mechanics-I (20 L):

Beginning of Quantum Mechanics:

Black body radiation, photoelectric and Compton effects, light as stream of particles; wave-particle duality, electrons and waves, de Broglic equation and matter wave, Uncertainty relations (without proof), principle of complimentarity.

Concepts of operators:

Elementary concepts of operators, eigen functions and eigen values, linear and non-linear operators, commutation of operators, commutator and uncertainty relation, Expectation value, properties of Hermitian operators.

Wave functions: Postulates of Quantum Mechanics, Schrodinger equation, nature of equation, acceptability conditions for the wave functions and probability interpretations of the wave functions.

Quantization of translation motion:

Schrödinger equation for a free particle in a one-dimensional box and its energy eigen values (E_n) and wave functions ($\Psi_n(x)$), Comparison with free particle eigen functions and eigen values, properties of $\Psi_n(x)$ (normalization, orthogonality, probability distribution), expectation values of x, x^2 , p_x and p_x^2 and their significance in relation to the uncertainty principle, extension of the problem to two and three dimensions and concept of degenerate energy levels.

Tunneling concept:

Tunneling of a particle through a potential barrier.

Solid state (10 L):

The nature of solid state, coefficient of thermal expansion, thermal compressibility of solids, Dulong-Petit Law, Amorphous and crystalline solids; Perfect crystals (lattice + basis), law of constancy of interfacial angles, concept of unit cell, crystal systems, Bravais lattices, law of rational indices, Weiss & Miller indices, interplanar distance, packing fraction; symmetry elements in crystals and Quasi-crystals.

X-Ray diffraction, Bragg's law, Laue's method, Powder method, Brief ideas about electron & Neutron diffraction, crystal structure of NaCl and KCl, radius ratios rule and packing in crystals.

Laboratory Experiments :

Paper : Chem/PR/05 : (2 Credit, FM-50, 4 L/W; 60L)

Unit : 305L-I : Inorganic Chemistry-II

Separation of Mixtures

- 1. Estimation of Cu(II).
- 2. Estimation of Fe(III) and Mn(II) in a mixture using standardized KMnO4 solution.
- 3. Estimation of Fe(III) and Cu(II) in a mixture using K₂Cr₂O₇.
- 4. Estimation of Fe(III) and Cr(III) in a mixture using $K_2Cr_2O_7$.
- 5. Estimation of Fe(III) and Ca(II) in a mixture.

Paper : Chem/PR/06 : (2 Credit, FM-50, 4 L/W; 60L)

Unit : 306L-P: Physical Chemistry-II

List of Experiments

- 1. Determination of the surface tension of supplied liquid by capillary rise method.
- 2. Determination of the strength of supplied solution from the plot of 'viscosity coefficient' vs. 'concentration of solution'.
- 3. Determination of rate constants of acid catalyzed hydrolysis methyl acetate at two acid concentrations.
- 4. Determination of rate constants of KI catalyzed decomposition of hydrogen peroxide at two KI concentrations using clock method.
- 5. Study of the distribution of benzoic acid between benzene and water.
- 6. Study of the kinetics of iodination of acetone.

Paper : Chem/PR/07 : (2 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 307L-P : Physical Chemistry-III</u>

- 1. Determination of the K_c of the reaction: $CH_3COOH(aq) + C_2H_5OH(aq) \implies CH_3COOC_2H_5(aq) + H_2O(l)$.
- 2. Determination of the specific rotation of sucrose and strength of its supplied solution.
- 3. Verification of Freundlich Adsorption Isotherm.

- 4. Determination of K_C of the reaction: $KI + I_2 \implies KI_3$ by partition method.
- 5. Determination of molar extinction coefficient of $K_2Cr_2O_7$ and strength of its solution.
- 6. Determination of the order of alkaline fading of crystal violet with respect to alkali and crystal violet, colorimetrically.

Semester -IV

Theory Papers :

Paper: Chem/TH/08 : (4 Credit, FM-50, 4 L/W; 60L) <u>Unit : 4081-I</u> : Coordination Chemistry – I; Molecular symmetry and Point Groups (30L):

Coordination Chemistry – I (15 L):

Werner's theory – Concept of primary and secondary valency, explanation of structures of cobalt ammines(hexacoordinate) by Werner's theory.

Classification of ligands, IUPAC nomenclature of coordination compounds including the polynuclear ones. Configuration index. Structure of coordination compounds from orbital hybridization of central atoms – linear (sp), square planar (dsp^2), tetrahedral (sp^3 , d^3s), trigonal bipyramidal (dsp^3), octahedral (d^2sp^3) etc. with examples. Isomerism: Stereoisomerism (Geometrical and optical) and Constitutional in square planar and octahedral complexes. Stability of complex ions in solution – various factors; 'the chelate effect'. Approach to preparation of coordination compounds – by substitution reactions in aq. solution and non aq. solution, 'the *trans* effect' and synthesis of all possible isomers.

Molecular symmetry and Point Groups (15 L):

The concept of symmetry in three dimensional objects, in molecules, Symmetry elements and symmetry operations – C_n , S_n , σ_h , σ_v , σ_d , i, E. Finding the complete collection of the symmetry elements (of various orders) in molecules and regular polyhedra (tetrahedron, octahedron, cube, icosahedrons), reduction in symmetry on substitution in molecules or on deformation of regular polyhedra.

Classification of molecules according to symmetry elements present into point groups. Schoenflies notations for the point groups. Symmetry of orbitals (Mulliken Notation). Systematic identification of point groups of various molecules. Examples.

<u>Unit : 4082-I</u> : Chemistry of p- Block Elements (30 L):

Chemistry of p- Block Elements:

General group properties (*) :

For each group these include discussion on a comparative basis of major physical and chemical properties like,

i) Common natural sources of the elements.

ii) Physical properties – the electronic configuration; ionisation potential / electron affinity; m.p., b.p.; ionic / covalent radii etc.

iii) Chemical properties – Various oxidation states and their relative stability (redox behaviour in solution, wherever applicable), higher stability of the higher oxidation states for the heavier members; gradual changes of the ionic/covalent character of the compounds from lighter to heavier members; the relative acidity, amphoteric, basic characteristics of the oxides and formation of oxocations (wherever applicable); examples of compounds in all the oxidation states, in particular, the unusual (rare) oxidation states being stabilized through coordination; hydrides, halides (including the halo complexes) and their hydrolytic behaviour; dimerization and/or polymerization through halogen bridges (wherever applicable) etc.

Gr. 13.

(a) General group properties (* as described above).

(b) Boron Chemistry – preparation, properties of boranes; Structure and bonding of diborane, Borazine, Boron nirides; electron deficient nature of hydrides, halides and their polymerisation.

Gr. I4

(a) General group properties (* as described above).

(b) Intercalation compounds e.g. Graphite Intercalation compounds (GIC), CNT (Carbon Nanotube), graphenes and fullerenes.

(c) Preparation, properties and uses of the fluorocarbons, the silanes, sillicates and the silicones.

Gr. 15

(a) General group properties (* as described above).

(b) The presence of lone pair and basicity of trivalent compounds; trends in bond angles of hydrides, halides, preparation, properties, structures and bonding of hydrazine, hydroxylamine, hydrazoic acids, the oxides and oxyacids of N, P; Phosphazene, phosphonirtilic compounds $(PNCl_2)_n$.

Gr. 16

(a) General group properties (* as described above).

(b) Preparation, properties, structures and bonding of the oxides, oxyacids (including the thionous, thionic and peracids) of sufur, halides, oxy-halides and poly sulphides; sulfur nitrogen compounds $(SN)_x$.

Gr. 17

(a) General group properties (* as described above).

(b) Color of Halogens in different medium. Halogen hydrides, their acidity; Preparation, properties, structures and bonding of the oxides and oxy acids; Clathrate compounds.

(c) Synthesis, structures and properties of (i) the inter-halogen compounds, (ii) polyhalogen ions [isopoly & heteroploy halogen cations and isopoly & heteroploy halogen anions] and pseudohalides including their preparations, properties and structures.

Paper: Chem/TH/09 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 4091-O</u> : Nitrogen compounds; Rearrangements (30L):

A. Nitrogen compounds (15 L) :

- 1. Amines: Aliphatic & Aromatic: preparation, separation (Hinsberg's method) and identification of primary, secondary and tertiary amines; reaction (with mechanism): Eschweiler–Clarke methylation, diazo coupling reaction, Mannich reaction; formation and reactions of phenylenediamines, diazomethane and diazoacetic ester.
- 2. Nitro compounds (aliphatic and aromatic): Preparation and reaction (with mechanism): reduction under different conditions; Nef carbonyl synthesis.
- **3.** Alkylnitrile and isonitrile: Preparation and reaction (with mechanism): Thorpe nitrile condensation, von Richter reaction.
- 4. Diazonium salts and their related compounds: Peactions (with mechanism) involving replacement of diazo group; reactions: Gomberg, Meerwein, Japp-Klingermann.

B. Rearrangements (15 L):

Mechanism with evidence and stereochemical features for the following:

- 1. Rearrangement to electron-deficient carbon: Wagner-Meerwein rearrangement, pinacol rearrangement, dienone-phenol; Wolff rearrangement in Arndt-Eistert synthesis, benzil-benzilic acid rearrangement, Demjanov rearrangement, Favorski rearrangement.
- 2. Rearrangement to electron-deficient nitrogen: rearrangements: Hofmann, Curtius, Lossen, Schmidt and Beckmann.
- **3. Rearrangement to electron-deficient oxygen**: Baeyer-Villiger oxidation, cumene hydroperoxide-phenol rearrangement and Dakin reaction.
- 4. Aromatic rearrangements: Migration from oxygen to ring carbon: Fries rearrangement and Claisen rearrangement.
- 5. Migration from nitrogen to ring carbon: Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, *N*-azo to *C*-azo rearrangement, Bamberger rearrangement, Orton rearrangement and benzidine rearrangement.

<u>Unit : 4092-O</u> : The Logic of Organic Synthesis; Organic Spectroscopy (30L):

The Logic of Organic Synthesis (15 L):

1. Retrosynthetic analysis: Disconnections; synthons, donor and acceptor synthons; natural reactivity and umpolung; latent polarity in bifunctional compounds: consonant and dissonant polarity; illogical electrophiles and nucleophiles; synthetic equivalents; functional group interconversion and addition (FGI and FGA); C-C disconnections and synthesis: one-group and two-group (1,2- to 1,5-dioxygenated compounds), reconnection (1,6-dicarbonyl); protection-deprotection strategy (alcohol, amine, carbonyl, acid).

- 2. Strategy of ring synthesis: Thermodynamic and kinetic factors; synthesis of large rings, application of high dilution technique.
- **3.** Asymmetric synthesis: Stereoselective and stereospecific reactions; diastereoselectivity and enantioselectivity (only definition); enantioselectivity: kinetically controlled MPV reduction; diastereoselectivity: addition of nucleophiles to C=O adjacent to a stereogenic centre: Cram, Felkin-Anh and Prelog models.

Organic Spectroscopy (15 L):

- 1. UV Spectroscopy: Introduction; types of electronic transitions, end absorption; transition dipole moment and allowed/forbidden transitions; chromophores and auxochromes; Bathochromic and Hypsochromic shifts; intensity of absorptions (Hyper-/Hypochromic effects); application of Woodward's Rules for calculation of λ max for the following systems: conjugated diene, α , β -unsaturated aldehydes and ketones (alicyclic, homoannular and heteroannular); extended conjugated systems (dienes, aldehydes and ketones); relative positions of λ_{max} considering conjugative effect, steric effect, solvent effect, effect of pH; effective chromophore concentration: keto-enol systems; benzenoid transitions.
- IR Spectroscopy: Introduction; modes of molecular vibrations (fundamental and non-fundamental); IR active molecules; application of Hooke's law, force constant; fingerprint region and its significance; effect of deuteration; overtone bands; vibrational coupling in IR; characteristic and diagnostic stretching frequencies of C-H, N-H, O-H, C-O, C-N, C-X, C=C (including skeletal vibrations of aromatic compounds), C=O, C=N, N=O, C=C, C≡N; characteristic/diagnostic bending vibrations are included; factors affecting stretching frequencies: effect of conjugation, electronic effects, mass effect, bond multiplicity, ring-size, solvent effect, H-bonding on IR absorptions; application in functional group analysis.
- 3. NMR Spectroscopy: Introduction; nuclear spin; NMR active molecules; basic principles of Proton Magnetic Resonance; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect; significance of the terms: up-/downfield, shielded and deshielded protons; spin coupling and coupling constant (1st order spectra); relative intensities of first-order multiplets: Pascal's triangle; chemical and magnetic equivalence in NMR; elementary idea about non-first-order splitting; anisotropic effects in alkene, alkyne, aldehydes and aromatics; NMR peak area, integration; relative peak positions with coupling patterns of common organic compounds (both aliphatic and benzenoid-aromatic); rapid proton exchange; interpretation of NMR spectra of simple compounds.
- 4. Applications: IR, UV and NMR spectroscopy for identification of simple organic molecules.

Paper: Chem/TH/10 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 4101-P</u> : Colligative Properties & Phase Equilibria (30L) :

Colligative Properties (using concept of chemical potential):

Different physical properties of liquid solvent, dilute solution, ideally dilute solution, Raoult's law & Henry's law, lowering & relative lowering of vapour pressure, elevation of boiling point, depression of freezing point, osmosis, osmotic pressure and its determination, relation between colligative properties and molecular mass, van't Hoff factor, abnormal colligative properties.

Phase Equilibria:

Equilibria among different phases, phase, component, degree of freedom, derivation of Gibbs phase rule for non-reactive and reactive systems.

Nernst distribution law & solvent extraction principle, steam distillation, phase diagrams of one-component systems (water, carbon dioxide & sulfur), triple point, derivation of Duhem-Margules rule & Konowaloff rule, phase diagram of liquid pair (partially miscible & completely miscible), Lever Rule, upper & lower critical solution temperature, azeotropic mixture, isobaric fractional distillation, phase diagram of two-component systems (solid-solution equilibrium) involving simple eutectics and compound with congruent & incongruent melting points, eutectic mixture, fractional crystallization, peritectic point and peritectic change, cooling curves and phase diagrams.

Phase diagram of 3-component systems (with example of glacial acetic acid, water & benzene).

<u>Unit : 4102-P</u> : Transport Properties, Conductance & Ionic equilibria (20L); Photochemistry-I (10L)

Transport Properties: Fick's law (Flux and Force), Phenomenological coefficients & their inter-relationship, different examples of transport properties.

Conductance: Ion conductance; Conductance and measurement of conductance, cell constant, conductivity, equivalent conductivity and molar conductivity; Variation of conductivity and equivalent conductivity with dilution for true and potential electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductivity at infinite dilution and their determination for true and potential electrolytes; Debye–Huckel theory of Ion atmosphere (qualitative)-asymmetric effect and electrophoretic effect; dependence of activity coefficient on ionic strength, Ostwald's dilution law; Ionic mobility; Solubility equilibrium and Solubility product; Application of conductance measurement, determination of solubility product, ionic product of water and dissociation constants of acids and bases; conductometric titrations; Transport number, Principles of Hittorf's and Moving-boundary method; Wien effect, Debye-Falkenhagen effect, Walden's rule. Anomalous transference numbers, proton jump mechanism, ionic mobility and absolute mobility, Nernst – Einstein equation.

Ionic equilibria:

Chemical potential of an ion in solution; Activity and activity coefficients of ions in solution; Brief qualitative description of the model and the postulates involving Debye-Hückel limiting law, the equation (without derivation) for ion-ion interaction.

Photochemistry-I (10 L):

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, absorption, molar extinction coefficient and its physical significance. modification of electronic and molecular properties of molecules upon photoexcitation. Franck Condon principle, Luminescence: resonance radiation, fluorescence, phosphorescence, chemiluminescence; Jablonski diagram, singlet and triplet states, decays of excited states by radiative and non-radiative pathways, internal conversion (IC) and intersystem crossing (ISC), quenching of fluorescence, Stern-Volmer equation: derivation, its application and limitation.

Paper: SEC/Chem/02 : (2 Credit, FM-50, 2 L/W; 30 L):

<u>Unit : SEC02-1</u> : Errors in Chemical Analysis; Use of Organic Reagents; Analysis of Soil; Analysis of Water, Food Products, Cosmetics and Other Applications.

A. Errors in Chemical Analysis; Use of Organic Reagents; Analysis of Soil (15 L):

(i) Errors in Chemical Analysis

Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy and precision of quantitative analysis, determinate, indeterminate, systematic and random errors; methods of least squares and standard deviations. Propagation of errors; presentation of experimental data and results, from the point of view of significant figures.

(ii) Use of Organic Reagents

Criteria for choice of organic reagents, use of following reagents in inorganic analysis: DMG, cupferron, 8-hydroxy-quinoline, Nitroso α -naphthol, EDTA, Acetylacetone, dithiozone, dithiocarbamate. Advantages and disadvantages of organic reagents in inorganic analysis.

(iii) Analysis of Soil

Composition of soil, concept of pH and pH measurement.

- 1. Determination of pH of soil samples.
- 2. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

B. Analysis of Water, Food Products, Cosmetics and Other Applications (15 L):

(i) Analysis of Water

Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.

- 1. Determination of pH, acidity and alkalinity of a water sample.
- 2. Determination of dissolved oxygen (DO), BOD and COD of water sample.

(ii) Analysis of Food Product

Nutritional value of foods, idea about food processing and food preservations and adulteration.

- 1. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
- 2. Analysis of preservatives and colouring matter.

(iii) Analysis of Cosmetic

Major and minor constituents and their function.

1. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.

2. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

(iv) Other Applications

- 1. To study the use of phenolphthalein in trap cases.
- 2. To analyse arson accelerants.
- 3. To carry out analysis of gasoline.

Laboratory Experiments :

Paper : Chem/PR/08: (2 Credit, FM-50, 4 L/W; 60L)

Unit : 408L-I : Inorganic Chemistry-III

Inorganic preparations:

- 1. Potassium tris(oxalate)ferrate(III).
- 2. Tris-(ethylenediamine) nickel(II) chloride.
- 3. $[Mn(acac)_3]$ and $Fe(acac)_3]$ (acac= acetylacetonate).

Complexometric titration:

- 1. Zn(II).
- 2. Zn(II) and Cu(II) mixture.
- 3. Ca(II) and Mg(II) in a mixture.
- 4. Hardness of water.
- 5. Estimation of amount of iron and oxalic present in Potassium tris(oxalate)ferrate(III).

Paper : Chem/PR/09 : (2 Credit, FM-50, 4 L/W; 60L)

Unit : 409L-O : Organic Chemistry-III

Qualitative Analysis of Single Solid Organic Compounds

- 1. Detection of special elements (N, S, Cl, Br) by Lassaigne's test using metallic sodium and zinc-sodium carbonate.
- 2. Solubility and classification (solvents: H₂O, 5% HCl, 5% NaOH and 5% NaHCO₃).
- Detection of the following functional groups by systematic chemical tests: Aromatic amino (-NH₂), aromatic nitro (-NO₂), amido (-CONH₂, including imide), phenolic –OH, carboxylic acid (-COOH), carbonyl (-CHO and >C=O); (*only one test for each functional group is to be reported*).
- 4. Melting point of the given compound.
- 5, Preparation, purification and melting point determination of a crystalline derivative of the given compound.
- 7. Identification of the compound through literature survey.

Each student, during laboratory session, is required to carry out qualitative chemical tests for all the special elements and the functional groups with relevant derivatisation in known and unknown (at least six) organic compounds

Paper : Chem/PR/10 : (2 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 410L-O</u> : Organic Chemistry-IV

Organic Quantitative analysis :

- 1. Estimation of glycine by Sörensen's formol method.
- 2. Estimation of glucose by titration using Fehling's solution.
- 3. Estimation of sucrose by titration using Fehling's solution.
- 4. Estimation of vitamin-C (reduced).
- 5. Estimation of aromatic amine (aniline) by bromination (Bromate-Bromide) method .
- 6. Estimation of phenol by bromination (Bromate-Bromide) method .
- 7. Estimation of formaldehyde (Formalin).
- 8. Estimation of acetic acid in commercial vinegar.
- 9. Estimation of urea (hypobromite method).
- 10. Estimation of saponification value of oil/fat/ester.

Theory Papers :

Paper: Chem/TH/11: (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 5111- I</u> : Coordination Chemistry; Colour, Magnetism and Bioinorganic Chemistry (30L) : A. Coordination Chemistry – II (15 L):

- i) Basic principles, splitting of d-orbital degeneracy due to electrostatic field of various symmetry-octahedral, tetrahedral, tetragonally distorted octahedral, square planar, trigonal bipyramid.
- ii) Strong field, weak field cases and high spin-low spin electronic configurations in Oh, T_d symmetry. Spectrochemical series.
- iii) Crystal field stabilisation energy (CFSE) in O_h and T_d field, the manifestation of CFSE.
- iv) OSSE. Normal and inverted spinel structures
- v) Jahn–Teller theorem and the Jahn–Teller distortion in d^1-d^9 systems in Oh and Td fields.
- vi) Limitations of the crystal field model; evidences in favour of metal-ligand bonding. Nephelauxetic effects. Ligand Field Theory.
- vii) Qualitative Treatment of Molecular Orbital Theory: sigma and pi-bonding in octahedral complexes (pictorial approach) and their effects.

B. Colour, Magnetism and Bioinorganic Chemistry (15L):

i) Colour (7 L):

L-S coupling; d-d transition, Orgel diagrams for $3d^1$ to $3d^9$ ions (excluding d^5). Racah parameter. Selection rules for electronic spectral transitions; charge transfer spectra (elementary idea).

ii) Magnetism (3 L):

Orbital and spin magnetic moments, spin only moments of dⁿ ions and their correlation with effective magnetic moments, Spin state isomerism, orbital contribution; quenching of magnetic moment: direct exchange interaction: super exchange interactions (elementary idea with examples).

iii) Bioinorganic Chemistry (5 L):

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Na-/ K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, use of chelating agents in medicine. Iron and its application in bio-systems, Haemoglobin and Myoglobin: storage and transfer of oxygen.

<u>Unit : 5112- I</u> : Transition Elements and Lanthanoids and Actinoids (30L):</u>

Transition Elements (22L) :

General comparison of 3d, 4d and 5d elements in terms of electronic configuration, relativistic effect, oxidation states, redox properties; coordination chemistry of various oxidation states.

Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy), $K_2Cr_2O_7$, $KMnO_4$, $K_3[Fe(CN)_6]$, $K_4[Fe(CN)_6]$, Prussian blue.

Lanthanoids and Actinoids (8 L) :

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanoides (ion-exchange method only).

Paper: Chem/TH/12 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 5121- O</u> : Carbocycles, Heterocycles and Cyclic Stereochemistry (30L):

1. Polynuclear hydrocarbons and their derivatives (5 L):

Synthetic methods include Haworth, Bardhan-Sengupta, Bogert-Cook and other useful syntheses (with mechanistic details); fixation of double bonds and Fries rule; reactions (with mechanism) of naphthalene, anthracene, phenanthrene and their derivatives.

2. Heterocyclic compounds (10 L):

5- and 6-membered rings with one heteroatom; reactivity, orientation and important reactions (with mechanism) of furan, pyrrole, thiophene and pyridine; synthesis (including retrosynthetic approach and mechanistic details): pyrrole: Knorr synthesis, Paal-Knorr synthesis, Hantzsch; furan: Paal-Knorr synthesis, Feist-Benary synthesis and its variation; thiophenes: Paal-Knorr synthesis, Hinsberg synthesis; pyridine: Hantzsch synthesis; benzo-fused 5- and 6-membered rings with one heteroatom: reactivity, orientation and important reactions (with mechanistic details) of indole, quinoline and isoquinoline; synthesis (including retrosynthetic approach and mechanistic details): indole: Fischer, Madelung and Reissert; quinoline: Skraup, Doebner- Miller, Friedlander; isoquinoline: Bischler-Napieralski synthesis.

3. Cyclic Stereochemistry (15 L):

Concept of I-strain; conformational analysis: cyclohexane, mono and disubstituted cyclohexane; symmetry properties and optical activity; topomerisation; ring-size and ease of cyclisation; Baldwin rules for ring forming reactions, conformation & reactivity in cyclohexane system: consideration of steric and stereoelectronic requirements; elimination (E2, E1), nucleophilic substitution (S_N1 , S_N2 , S_N^i , NGP), merged substitution-elimination; rearrangements; oxidation of cyclohexanol, esterification, saponification, lactonisation, epoxidation, pyrolytic syn elimination and fragmentation reactions.

Resolution of acids, bases and alcohols via diastereomeric salt formation; optical purity and enantiomeric excess; invertomerism of chiral trialkylamines.

<u>Unit : 5122- O</u> : Pericyclic reactions and Biomolecules (30L) :

A. Pericyclic reactions (15 L):

Mechanism, stereochemistry, regioselectivity in case of

- 1. Electrocyclic reactions: Frontier Molecular Orbital (FMO) approach involving 4π and 6π -electrons (thermal and photochemical) and corresponding cycloreversion reactions.
- 2. Cycloaddition reactions: FMO approach, Diels-Alder reaction, photochemical [2+2] cycloadditions.
- **3.** Sigmatropic reactions: FMO approach, sigmatropic shifts and their order; [1,3]- and [1,5]-H shifts and [3,3]- shifts with reference to Claisen and Cope rearrangements.

B. Biomolecules (15L):

1. Carbohydrates: (6L)

Monosaccharides: Aldoses up to 6 carbons; structure of D-glucose & D-fructose (configuration & conformation); ring structure of monosaccharides (furanose and pyranose forms): Haworth representations and non-planar conformations; anomeric effect (including stereoelectronic explanation); mutarotation; epimerization; reactions (mechanisms in relevant cases): Fischer glycosidation, osazone formation, bromine-water oxidation, HNO₃ oxidation, selective oxidation of terminal –CH₂OH of aldoses, reduction to alditols, Lobry de Bruyn-van Ekenstein rearrangement; stepping–up (Kiliani-Fischer method) and stepping–down (Ruff's &Wohl's methods) of aldoses; end-group-interchange of aldoses; acetonide (isopropylidene) and benzylidene protections; ring-size determination; Fischer's proof of configuration of (+)-glucose.

Disaccharides: Glycosidic linkages, concept of glycosidic bond formation by glycosyl donor-acceptor; structure of sucrose, inversion of cane sugar.

2. Amino acids, peptides and nucleic acids: (5 L)

- **a.** Amino acids: Strecker, Gabriel, acetamidomalonic ester, azlactone, Bücherer hydantoin isoelectric point, zwitterions; electrophoresis, reaction with ninhydrin.
- b. Peptides and Nucleic acids (elementary idea).

3. Pharmaceutical Compounds: (4 lectures)

Classification, structure and therapeutic uses of: i) antipyretics: Paracetamol (with synthesis), ii) analgesics: Ibuprofen and aspirin (with synthesis), and iii) antimalarials: Chloroquine (with synthesis). An elementary treatment of antibiotics (study of Chloramphenicol), antibacterial and antifungal agents (Sulphonamides and Sulphacetamide), central nervous system agents (Diazepam) and antiviral agent (Acyclovir).

Paper: Chem/TH/13 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 5131- P</u> : Adsorption & Colloids; Nanomaterials; Polymer (30L):

Adsorption & Colloids (15 L):

Physisorption and chemisorption, adsorption isotherms, quantitative aspects of Freundlich and Langmuir adsorption isotherms; BET equation and its use in surface area determination, adsorption and heterogeneous catalysis.

Colloids (Lyophilic and Lyophobic), electrical double layer and colloid stability, Protective action, Gold number' electrokinetic phenomena, elementary ideas about soaps and detergents, micelles and emulsions;.

Pressure inside a droplet, vapour pressure of curved surfaces and Kelvin's equation, concept of surface excess, Gibbs equation insoluble monolayer and surface pressure. Liquid- liquid interface-immiscibility, contact angle and surface spreading.

Nanomaterials & Polymer (15 L):

Definition and different types of nanomaterials. Different types of synthesis of nanomaterials and their advantages. Characterization of nanomaterials by different techniques (explanation only). Different properties and size effect. Nanoaggregates, carbon nanotubes and their classification.

Characteristics of macromolecules, polymerization, types of polymerization, degree of polymerization, concept of number and mass average relative molecular mass, osmometry, viscometry, light scattering and diffusion methods in the studies of average relative molecular masses and shapes of macromolecules.

<u>Unit : 5132- P</u> : Electrochemistry (30 L):

Electromotive Force:

Rules of oxidation/ reduction of ions based on half-cell potentials, Chemical cells, reversible and irreversible cells with examples; Electromotive force of a cell and its measurement, Nernst equation; Standard electrode, reduction potential and its application to different kinds of half-cells, construction of cells.

Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone and glass electrodes, determination of solubility product and ionic product of water, measurement of mean ionic activity coefficient of electrolytes, determination of E° of M^{z+}/M systems, activity coefficients of HX, MX etc. Determination of pK_a and pK_b of acids, bases and of ampholytes by emf methods, Brief descriptions of electrochemical power sources; primary, secondary, Lithium batteries and fuel cells.

Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers; Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).

Polarization and overvoltage phenomena, Activation polarization; basics of activation controlled reactions, Tafel Equation. Preliminary ideas of cyclic voltammetry, corrosion and inhibition of corrosion and electroplating, applications of electrolysis in metallurgy and industry.

Paper: Chem/TH/14: (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 5141- I</u> : Organometallics; Coordination Chemistry of Nontransition elements and Inorganic Reaction Mechanism (30L):

A. Organometallics (15L) :

Definition and classification of organometallic compounds on the basis of bond type, 18-electron and 16-electron rules (MO Theory) and their applications to carbonyls (including carbonyl hydrides and carbonylates), nitrosyls, cyanides, and nature of bonding involved therein. General methods of preparation of mono and binuclear carbonyls of 3d series. Structures of mono nuclear and binuclear carbonyls, pi-acceptor behaviour of CO, synergic effect and use of IR data to explain the extent of back bonding.

Hapticity (η) of organometallic ligands, examples of mono, tri- and tetra, penta, hexa, hepta and octa-haptocomplexes.

Metal- olefin complexes: Zeise's salt (preparation, structure and bonding). Ferrocene (preparation, structure and reactions).

B. Coordination Chemistry of Nontransition elements and Inorganic Reaction Mechanism (15L): (a) Coordination Chemistry of Nontransition elements :

- (i) Group I, II, III Complexes (other than those with aqua and hydroxo ligands). Preference for donor atoms selection of donor sites in biological systems. Complexes (where applicable) with monodentate and polydentate ligands halides, nitrates, alkoxides, carboxylates, aminopolycarboxylates, polyhydroxy compounds, betadiketones, 8–quinolinol,
- (ii) Complexes of B, Si, As, Sb, Te, Br and I (wherever applicable) with N and O –donor ligands with emphasis on cationic chemistry.
- (iii) Stereochemistry of the complexes and their uses in analysis and medicine (e.g., tartaremetic, valinomycin etc.)

(b) Inorganic Reaction Mechanism:

Introduction to inorganic reaction mechanisms. Substitution reactions in octahedral complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes.

Unit : 5142-P : Quantum Mechanics-II; Electrical & Magnetic Properties of Materials (30L) :

Quantum Mechanics – II (20 L):

Quantization of vibrational motion: Qualitative treatment of simple harmonic oscillator model, setting up of Schrödinger equation and discussion of eigen values and wave functions, vibrational selection rule.

Angular momentum: Commutation rules, quantization of total and z-component angular momentum, Rigid rotator model of rotation of diatomic molecules, Schrödinger equation, transformation to polar coordinates, separation of variables, Spherical Harmonics, Discussion of solution.

Qualitative treatment on H-atom and H-like atom: Setting up of Schrödinger equation in Spherical polar coordinates, radial part, quantization of energy (only final energy expression), Average and most probable distances of electron from nucleus.

Valance bond and molecular orbital approaches: LCAO-MO treatment of H_2^+ , bonding and antibonding orbitals, qualitative extension to H_2 , comparison of LCAO-MO and VB treatments of H_2 (details not required).

Electrical & Magnetic Properties of Materials (10 L):

Basic idea of electrostatics, Dipole moments, and of bonds, electrostatics of dielectric media, Polarization and polarizability, Permittivity, Clausius–Mossotti equation, Debye equation, Lorentz-Lorentz equation; Ionic character of diatomic molecules, Bond Moments and Group moments, Applications of dipole moments; Diamagnetism and paramagnetism, magnetic susceptibility and its measurement.

Laboratory Experiemnts :

Paper : Chem/PR/11 : (2Credit, FM-50, 4 L/W; 60L) & Chem/PR/12 : (2 Credit, FM-50, 4 L/W; 60L) :

Unit : 511L-I (60L) & 512L-I (60L) : Inorganic Chemistry-IV

Qualitative semimicro analysis of mixtures containing four radicals. Emphasis should be given to the understanding of the chemistry of different reactions and to assign the most probable composition.

Cation Radicals: Na⁺, K⁺, Ca²⁺, Sr²⁺, Ba²⁺, Al³⁺, Cr³⁺, Mn²⁺/Mn⁴⁺, Fe³⁺, Co²⁺/Co³⁺, Ni²⁺, Cu²⁺, Zn²⁺, Pb²⁺, Bi³⁺, Sn²⁺/Sn⁴⁺, Sb^{3+/5+}, NH₄⁺, Mg²⁺.

Anion Radicals: F^- , Cl^- , Br^- , I^- , SCN^- , S^{2-} , SO_4^{2-} , NO_3^- , NO_2^- , PO_4^{3-} , AsO_4^{3-} , BO_3^{3-} , CrO_4^{2-} Insoluble Materials: $Al_2O_3(ig)$, $Fe_2O_3(ig)$, $Cr_2O_3(ig)$, SnO_2 , $SrSO_4$, $BaSO_4$, CaF_2 , $PbSO_4$.

Paper : Chem/PR/13 : (2 Credit, FM-50, 4 L/W; 60L)

Unit : 513L-O : Organic Chemistry-V

A. Chromatographic Separations

- 1. TLC separation of a mixture containing 2/3 amino acids.
- 2. TLC separation of a mixture of dyes (fluorescein and methylene blue).
- 3. Column chromatographic separation of leaf pigments from spinach leaves.
- 4. Column chromatographic separation of mixture of dyes.
- 5. Paper chromatographic separation of a mixture containing 2/3 amino acids.
- 6. Paper chromatographic separation of a mixture containing 2/3 sugars.

B. Spectroscopic Analysis of Organic Compounds

- 1. Assignment of labelled peaks in the 1H NMR spectra of the known organic compounds explaining the relative δ -values and splitting pattern.
- Assignment of labelled peaks in the IR spectrum of the same compound explaining the relative frequencies of the absorptions (C-H, O-H, N-H, C-O, C-N, C-X, C=C, C=O, N=O, C≡C, C≡N stretching frequencies; characteristic bending vibrations are included).
- 3. The students must record full spectral analysis of at least 15 (fifteen) compounds from the following list: (a) 4-Bromoacetanilide; (b) 2-Bromo-4'-methylacetophenone; (c) Vanillin; (d) 2-Methoxyacetophenone;
 - (e) 4-Aminobenzoic acid; (f) Salicylamide; (g) 2-Hydroxyacetophenone; (h) 1.3-Dinitrobenzene;
 - (i) Benzyl acetate; (j) trans-4-Nitrocinnamaldehyde; (k) Diethyl fumarate; (l) 4-Nitrobenzaldehyde;
 - (m) 4-Methylacetanilide; (n) Mesityl oxide; (o) 2-Hydroxybenzaldehyde; (p) 4-Nitroaniline ;
 - (q) 2-Hydroxy-3-nitrobenzaldehyde; (r) 2,3-Dimethylbenzonitrile; (s) Pent-1-yn-3-ol; (t) 3-Nitrobenzaldehyde;
 - (u) 3-Ethoxy-4-hydroxybenzaldehyde; (v) 2-Methoxybenzaldehyde; (w) Methyl 4-hydroxybenzoate;
 - (x) Methyl 3-hydroxybenzoate; (y) 3-Aminobenzoic acid; (z) Ethyl 3-aminobenzoate;

(aa) Ethyl 4-aminobenzoate; (bb) 3-Nitroanisole; (cc) 5-Methyl-2-nitroanisole; (dd) 3-Methylacetanilide.

Paper : Chem/PR/14 : (2 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 514L-P</u> : Physical Chemistry-IV

- 1. Determination of individual strengths in a mixture of two acids conductrometrically.
- 2. Study kinetic study of the reaction: $K_2S_2O_8 + KI \rightarrow 2K_2SO_4 + I_2$, colorimetrically.
- 3. Determination of strength of supplied weak acid solution and its K_a potentiometrically.
- 4. Determination of rate constant of acid catalyzed inversion of cane sugar.
- 5. Determination of strength of supplied dibasic acid solution and its K_a values pH-metrically.
- 6. Study kinetics of the alkaline hydrolysis of ethyl acetate conductometrically.
- 7. Study and draw the phase diagram of phenol-water system.

Semester -VI

Theory Papers :

Paper: DSE/Chem/TH/01: (Choice Based Paper) (4 Credit, FM-50, 4 L/W; 60L) (any one Unit from 6011-1 and 6012-1 to be chosen)

Unit : 6011- I : Analytical Methods in Chemistry-I and Analytical Methods in Chemistry-II (60L)

Analytical Methods in Chemistry-I (Optical methods of analysis; Thermal and Electroanalytical methods) (30L) :

Optical methods of analysis (15 L):

- 1. Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.
- 2. UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;
- 3. Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enoltautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.
- 4. Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.
- Structural illustration through interpretation of data, effect and importance of isotope substitution.
- 5. Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, and detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

Thermal and Electroanalytical methods of analysis (15 L):

Theory of thermogravimetry (TG), basic principle of instrumentation, Techniques for quantitative estimation of Ca and Mg from their mixture.

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pK_a values.

Analytical Methods in Chemistry-II (Separation Techniques) (30L) : Separation Techniques (30 L):

Separation Techniques (30 L):

- 1. Solvent extraction: classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation.
- 2. Technique of extraction: batch, continuous and counter current extractions.
- 3. Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.
- 4. Chromatography: classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange.
- 5. Development of chromatograms: frontal, elution and displacement methods.
- 6. Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.
- 7. Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).

<u>Unit : 6012- I</u> : Instrumental Methods of Chemical Analysis (60L)

Introduction to Spectroscopic Methods of Chemical Analysis :

Recap of the spectroscopic methods covered in detail in the core chemistry syllabus: Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation. (4 L)

Molecular spectroscopy (16L) :

Infrared spectroscopy :

Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

UV-Visible/ Near IR – emission, absorption, fluorescence and photoaccoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoaccoustic, fluorescent tags).

Separation techniques (16L) :

Chromatography: Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis (use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis.

Immunoassays and DNA techniques

Mass spectroscopy: Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).

Elemental analysis (8L):

Mass spectrometry (electrical discharges).

Atomic spectroscopy: Atomic absorption, Atomic emission, and Atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

NMR Spectroscopy (4L) :

Principle, Instrumentation, Factros affecting chemical shift, Spin-coupling, Applications.

Electroanalytical Methods: Potentiometry & Voltammetry (4 L). Radiochemical Methods (4 L). X-ray analysis and electron spectroscopy (surface analysis) (4 L).

Paper: DSE/Chem/TH/02 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 6021- O</u> : Green Chemistry-I (30L) :

A. Introduction to Green Chemistry (4L):

Definition of Green Chemistry; Need for Green Chemistry; Goals of Green Chemistry; Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

B. Principles of Green Chemistry and Designing a Chemical synthesis (22 L):

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:

- **a.** Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products, Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
- **b.** Prevention/minimization of hazardous/ toxic products reducing toxicity. risk = (function) hazard \times exposure; waste or pollution prevention hierarchy.
- c. Green solvents- supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.
- d. Energy requirements for reactions alternative sources of energy: use of microwaves and ultrasonic energy.
- e. Selection of starting materials; avoidance of unnecessary derivatization careful use of blocking/protecting groups.
- **f.** Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
- **g.** Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.
- **h.** Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

C. Future Trends in Green Chemistry (4 L):

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co-crystal controlled solid state synthesis (C2S3); Green chemistry in sustainable development.

<u>Unit : 6022-O</u> : Green Chemistry-II (30L) :

Examples of Green Synthesis/ Reactions and some real world cases:

- **a.** Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis).
- **b.** Planning of green reaction: Aldol, Friedel-Crafts, Michael, Knoevenagel, Cannizzaro, benzoin condensation and Dieckmann condensation.
- c. Rearrangement reactions by green approach: Fries rearrangement, Claisen rearrangement, Beckmann rearrangement, Baeyer-Villiger oxidation.

- **d.** Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction.
- e. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine).
- **f.** Surfactants for carbon dioxide replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
- g. Designing of environmentally safe marine antifoulant.
- h. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
- i. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.
- **j.** Healthier Fats and oils by Green Chemistry: Enzymatic Inter esterification for production of no Trans-Fats and Oils.
- k. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting.

Paper: DSE/Chem/TH/03 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 6031- P</u> : Photochemistry-II; Spectroscopy (30L) :

Photochemistry-II (5 L)

Photochemical reactions, Laws of photochemistry, quantum yield, Photosensitized reactions, Photochemical equilibrium.

Spectroscopy (25 L)

Interaction of electromagnetic radiation with atoms and molecules and various types of spectra, Born-Oppenheimer approximation, condition of resonance and energy of absorption for various types of spectra, origin of atomic spectra.

Rotational spectroscopy

Rigid rotor model, energy levels and wave functions of various states, selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, effect of isotopic substitution on rotational spectroscopy, rotational spectra for non-rigid molecular systems.

Vibrational spectroscopy

Harmonic oscillator model, classical equation of vibration, zero-point energy and its significance, energy levels and wave functions, spectra of diatomic vibrating rotor, P, Q, R branches, anharmonicity, Morse potential and dissociation energy, fundamentals, overtones and hot bands, prediction and assignment of vibrational bands for linear and non-linear triatomic molecules.

Raman spectroscopy

Qualitative treatment of Raman effect, rotational and vibrational Raman spectra, effect of nuclear spin, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

ESR spectroscopy

Principle of ESR spectroscopy, hyperfine structure, ESR of simple radicals.

<u>Unit : 6032- P</u> : Statistical Thermodynamics (30 L)

Basic concepts

Limitations of classical thermodynamics, brief resumes of the concepts of distributions of energy and speed, macrostates, microstates, configurations, qualitative differences between classical and quantum particles, thermodynamic probability, concepts of ensembles, need of ensemble approach to statistical thermodynamics, concept of phase space, postulates of statistical thermodynamics, entropy and probability, the Boltzmann entropy formula.

Classical distribution

Boltzmann distribution, partition function and its physical significance, molecular partition functions, Maxwell's speed distribution, Gibbs paradox, thermodynamic properties of ideal gas, monatomic gases, statistical thermodynamics' definition of temperature.

Applications

Properties of diatomic gases (translational, rotational, vibrational, electronic contributions), Theory of specific heat of monatomic crystals: Einstein's theory, Characteristic temperature, its limitations and Debye's modification (T^3 -law, rigorous deduction not needed) with low and high temperature results.

Paper: DSE/Chem/TH/04 : (Choice Based Paper) (4 Credit, FM-50, 4 L/W; 60L)

(Among the 3 units, 6041-I/6042-O/6043-P, only one unit has to be chosen)

<u>Unit : 6041- I</u> : Industrial and Environment Chemistry (4 Credits)

Industrial Chemistry :

A. Glass, Cement and Ceramics (15 L):

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements. Quantitative Analysis of Cement

B. Catalysis and Chemical Explosive (15 L):

General principles and properties of catalysts, Deactivation or regeneration of catalysts. Homogenous catalysis (catalytic steps and examples) and heterogenous catalysis (catalytic steps and examples).

Study of the following industrial processes:

a. Alkene hydrogenation (Wilkinson's Catalyst); b. Hydroformylation; c. Wacker Process;

d. Synthetic gasoline (Fischer Tropsch reaction); e. Ziegler-Natta catalysis for olefin polymerization.

Phase transfer catalysts, application of zeolites as catalysts.

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

Environmental Chemistry (30 L):

(i) Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry; Environmental effects of ozone, Major sources of air pollution. Pollution by SO_2 , CO_2 , CO, NO_x , H_2S and other foul smelling gases. Methods of estimation of CO, NO_x , SO_x and control procedures. Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, acid rains. Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

(ii) The Hydrosphere: environmental role of water, natural water sources, water treatment for industrial, domestic and laboratory uses; water pollutants; action of soaps and detergents, phosphates, industrial effluents, agricultural runoff, domestic wastes; thermal pollution, radioactive pollution and their effects on animal and plant life; water pollution episodes: water pollution control measures : waste water treatment; chemical treatment and microbial treatment; water quality standards: DO, BOD, COD, TDS and hardness parameters; desalination of sea water : reverse osmosis, electrodialysis.

(iii) The Lithosphere: water and air in soil, waste matters and pollutants in soil, waste classification, treatment and disposal; soil pollution and control measures.

Unit : 6042- O : Polymer Chemistry (60L):

1. Introduction and history of polymeric materials (4L) :

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

- **2.** Functionality and its importance (6L) : Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bi-functional systems, Poly-functional systems.
- 3. Kinetics of Polymerization (8L) :

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

- 4. Crystallization and crystallinity (4L): Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.
- 5. Nature and structure of polymers (6L):

Structure Property relationships. (Mn, Mw, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index.

6. Glass transition temperature (Tg) and determination of Tg (4L):

Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg).

7. Polymer Solution (5L) :

Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

8. Properties of Polymer (18 L):

(Physical, Thermal, Flow & Mechanical Properties)

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, Polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

9. Biopolymers (5L): Polysaccharides pentides proteins and nucleic

Polysaccharides, peptides, proteins and nucleic acids.

<u>Unit : 6043- P</u> : Application of Computers in Chemistry (60):

Basics:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the FORTRAN language, FORTRAN keywords and commands, Logical and Relational operators. Simple programs using these concepts, debugging. Matrix addition and multiplications. Statistical analysis.

Numerical methods:

Roots of equations

Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.

Differential calculus

Numerical differentiation.

Integral calculus

Numerical integration (Trapezoidal and Simpson's rule), Probability distributions and mean values. Simultaneous equations Matrix manipulation: addition, multiplication. Gauss-Siedal method. Interpolation, extrapolation and curve fitting Handling of experimental data. Conceptual background of molecular modeling

Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

Laboratory Experiments :

Paper : DSE/Chem/PR/01 : (2 Credit, FM-50, 4 L/W; 60L)

Unit : 6011L-I : Inorganic Chemistry-V

1. Separation Techniques – Chromatography:

- (i) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R_f values.
- (ii) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their R_f values.
- (iii) Paper chromatographic separation of Fe^{3+} , Al^{3+} , and Cr^{3+} .

2. Solvent Extractions:

Separation of a mixture of Ni^{2+} & Fe²⁺ by complexation with DMG and extracting the Ni^{2+} -DMG complex in chloroform, and determination of its concentrations by spectrophotometry.

3. Analysis of soil:

- (i) Determination of pH of soil.
- (ii) Total soluble salt.
- (iv) Estimation of calcium, magnesium, phosphate, nitrate
- 4. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.
- 5. Determination of exchange capacity of cation exchange resins and anion exchange resins.

- 6. Spectrophotometry:
 - a. Determination of pK_a values of indicator using spectrophotometry
 - b. Determination of chemical oxygen demand (COD)
 - c. Determination of biological oxygen demand (BOD)

<u>Unit : 6012L-I :</u> Instrumental Methods of Chemical Analysis (60L) :

(At least 10 experiments from below to be performed)

- 1. Safety Practices in the Chemistry Laboratory.
- 2. Determination of the isoelectric pH of a protein.
- 3. Titration curve of an amino acid.
- 4. Determination of the void volume of a gel filtration column.
- 5. Determination of a Mixture of Cobalt and Nickel (UV/Vis spectroscopy).
- 6. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water).
- 7. IR Absorption Spectra (Study of Aldehydes and Ketones).
- 8. Determination of Calcium, Iron, and Copper in Food by Atomic Absorption Spectroscopy.
- 9. Quantitative Analysis of Mixtures by Gas Chromatography (i.e., chloroform and carbon tetrachloride).
- 10. Separation of Carbohydrates by HPLC.
- 11. Determination of Caffeine in Beverages by HPLC.
- 12. Potentiometric Titration of a Chloride-Iodide Mixture.
- 13. Cyclic Voltammetry of the Ferrocyanide/Ferricyanide Couple.
- 14. Nuclear Magnetic Resonance.
- 15. Use of fluorescence to do "presumptive tests" to identify blood or other body fluids.
- 16. Use of "presumptive tests" for anthrax or cocaine.
- 17. Collection, preservation, and control of blood evidence being used for DNA testing.
- 18. Use of capillary electrophoresis with laser fluorescence detection for nuclear DNA (Y chromosome only or multiple chromosome).
- 19. Use of sequencing for the analysis of mitochondrial DNA.
- 20. Laboratory analysis to confirm anthrax or cocaine.
- 21. Detection in the field and confirmation in the laboratory of flammable accelerants or Explosives.
- 22. Detection of illegal drugs or steroids in athletes.
- 23. Detection of pollutants or illegal dumping.
- 24. Fibre analysis.

Paper : DSE/Chem/PR/02 : (2 Credit, FM-50, 4 L/W; 60L)

Unit : 602L-O : Organic Chemistry-VI

Green Chemistry Practical:

(Experiments will be selected from the following list.)

- 1. Preparation and characterization of gold nanoparticles using tea leaves.
- 2. Preparation of biodiesel from vegetable / waste cooking oil.
- 3. Extraction of D-limonene from orange peel using liquid carbon dioxide.
- 4. Benzoin condensation using thiamine hydrochloride as a catalyst instead of potassium cyanide.
- 5. Solid state synthesis of benzilic acid from benzil.
- 6. Solid phase synthesis of azomethines from p-toluidine and vanillin.
- 7. Solvent-free aldol condensation between 3,4-dimethoxybenzaldehyde and cyclohexanone/1-tetralone.
- 8. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
- 9. Preparation and synthetic application of tetrabutylammonium tribromide.
- 10. "On-water" synthesis of Hantzsch dihydropyridine.
- 11. Solid phase redox reactions.
- 12. Green multicomponent synthesis.
- 13. Any other experiment related to this theme.

Paper : DSE/Chem/PR/03 : (2 Credit, FM-50, 4 L/W; 60L)

Unit: 603L-P: Physical Chemistry-V

- 1. Determination of strength of Mohr salt solution potentiometrically.
- 2. Determination of indicator constant of an acid-base indicator.
- 3. Determination of standard reduction potential of Ag⁺/Ag-electrode.

- 4. Determination concentration solubility product of BaSO₄ conductometrically.
- 5. Determination of CMC of CTAB tensiometrically.
- 6. Determination of rate constant of acid catalyzed mutarotation of α -D-glucose.
- 7. Study and draw the phase diagram of ternary system of water, benzene and glacial acetic acid.

Paper : DSE/Chem/PR/04 : (2 Credit, FM-50, 4 L/W; 60L)

(Choice Based Paper: One unit from I/O/P to be chosen according to Unit chosen in Paper DSE/04/Chem) Unit : 604L-I

Project and Seminar on relevant topics in Inorganic Chemistry

Unit: 604L-O

Seminar/ Review on relevant topics in Organic Chemistry

Unit: 604L-P : Application of Computers in Chemistry

Computer programs based on numerical methods for

- 1. Roots of equations : (e.g. Volume of van der Waals gas and comparison with ideal gas, pH of a week acid).
- 2. Numerical differentiation (e.g., change in pressure for small change in volume of van der Waals gas, potentiometric titrations).
- 3. Numerical integration (e.g., entropy / enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
- 4. Matrix operations. Application of Gauss-Siedel method in colorimetry.
- 5. Simple exercise using molecular visualization software.

Reference Books (Honours Level)

Inorganic Chemistry:

- 1. A Theoretical Approach to Inorganic Chemistry A. F. Williams
- 2. Orbital Interactions in Chemistry- Albright, Burdett und Whangbo
- 3. Orbitals In Chemistry: A Modern Guide For Students Victor M. S. Gil
- 4. Inorganic Chemistry: Principles of Structure and Reactivity- Huheey, Keiter, Keiter
- 5. Inorganic Chemistry Miessler, Fischer & Tarr
- 6. Concepts and Models of Inorganic Chemistry- Douglas, McDaniel, Alexander
- 7. Physical Inorganic Chemistry A Coordination Chemistry Approach-, S. F. A. Kettle
- 8. Organometallics, 3rd, Completely Revised and Extended Edition Christoph Elschenbroich
- 9. Inorganic Chemistry Gary Wulfsberg
- 10. Inorganic Chemistry- Nils Wiberg, A. F. Holleman
- 11. Inorganic Chemistry- Catherine Housecroft & Alan G. Sharpe
- 12. Chemistry of the Elements A. Earnshaw and Norman Greenwood
- 13. Essential Trends in Inorganic Chemistry D. M. P. Mingos
- 14. Modern Inorganic Chemistry William L. Jolly
- 15. Inorganic Chemistry-D. Shriver; M; Weller; T. Overton; F. Armstrong; J. Rourke
- 16. Inorganic Chemistry–James E. House
- 17. An Introduction to Inorganic Chemistry- Keith F. Purcell, John C. Kotz
- 18. Advanced Inorganic Chemistry- Wilkinson, Murillo, Bochmann, Cotton
- 19. Essentials of Nuclear Chemistry Hari Jeevan Arnikar
- 20. Group Theory for Chemists: Fundamental Theory and Applications- K. C. Molloy
- 21. Chemical Applications of Group Theory F. A. Cotton
- 22. General & Inorganic Chemistry R. P. Sarkar
- 23. Bioinorganic Chemistry Bertini, Gray, Lippard, Valentine
- 24. Bioinorganic Chemistry- A. K. Das

Analytical, Environmental and Industrial Chemistry:

- 1. Analytical Chemistry G. D. Christian, P. K. Dasgupta, K. A. Schug
- 2. Fundamentals of Analytical Chemistry, D. A. Skoog.
- 3. Basic Concepts of Analytical Chemistry S M Khopkar
- 4. Analytical Chemistry: A Chemist and Laboratory Technician's Toolkit Bryan M. Ham, Aihui MaHam
- 5. Exploring Chemical Analysis D. C. Harris
- 6. Vogel's Quantitative Chemical Analysis
- 7. Vogel's Qulititative Chemical Analysis
- 8. Environmental Chemistry Anil Kumar De

- 9. Environmental Chemistry Stanley Manahan
- 10. Industrial Chemistry B. K. Sharma
- 11. Engineering Chemistry Jain & Jain
- 12. Principles of Instrumental Analysis 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
- 13. Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.
- 14. C.N. Banwell: Fundamentals of Molecular Spectroscopy.
- 15. Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.

Organic Chemistry:

- 1. Clayden, J., Greeves, N. & Warren, S. Organic Chemistry, Second edition, Oxford University Press, 2012.
- 2. Sykes, P.A guidebook to Mechanism in Organic Chemistry, Pearson Education, 2003.
- 3. Smith, J. G. Organic Chemistry, Tata McGraw-Hill Publishing Company Limited.
- 4. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 5. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd., (Pearson Education).
- 6. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 7. Fleming, I. Molecular Orbitals and Organic Chemical Reactions, Reference/Student Edition, Wiley, 2009.
- 8. James, J., Peach, J. M. Stereochemistry at a Glance, Blackwell Publishing, 2003.
- 9. Robinson, M. J. T., Stereochemistry, Oxford Chemistry Primer, Oxford University Press, 2005.
- 10. Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London, 1994.
- 11. Nasipuri, D. Stereochemistry of Organic Compounds, Wiley Eastern Limited.
- 12. Carey, F. A. & Guiliano, R. M. Organic Chemistry, Eighth edition, McGraw Hill Education, 2012.
- 13. Loudon, G. M. Organic Chemistry, Fourth edition, Oxford University Press, 2008.
- 14. Graham Solomons, T.W., Fryhle, C. B. Organic Chemistry, John Wiley & Sons, Inc.
- 15. Maskill, H., Mechanisms of Organic Reactions, Oxford Chemistry Primer, Oxford University Press.
- 16. Norman, R.O. C., Coxon, J. M. Principles of Organic Synthesis, Third Edition, Nelson Thornes, 2003.
- 17. March, J. Advanced Organic Chemistry, Fourth edition, Wiley.
- 18. Jenkins, P. R., Organometallic Reagents in Synthesis, Oxford Chemistry Primer, Oxford University Press.
- 19. Ward, R. S., Bifunctional Compounds, Oxford Chemistry Primer, Oxford University Press.
- 20. Silverstein, R. M., Bassler, G. C., Morrill, T. C. Spectrometric Identification of Organic Compounds, John Wiley and Sons, INC, Fifth edition.
- 21. Kemp, W. Organic Spectroscopy, Palgrave.
- 22. Pavia, D. L. et al. Introduction to Spectroscopy, 5th Ed. Cengage Learning India Ed. (2015).
- 23. Dyer, J. Application of Absorption Spectroscopy of Organic Compounds, PHI Private Limited
- 24. Harwood, L. M., Polar Rearrangements, Oxford Chemistry Primer, Oxford University Press.
- 25. Bailey, Morgan, Organonitrogen Chemistry, Oxford Chemistry Primer, Oxford University Press.
- 26. Warren, S. Organic Synthesis the Disconnection Approach, John Wiley and Sons.
- 27. Warren, S., Designing Organic Synthesis, Wiley India, 2009.
- 28. Carruthers, W. Modern methods of Organic Synthesis, Cambridge University Press.
- 29. Willis, C. A., Wills, M., Organic Synthesis, Oxford Chemistry Primer, Oxford University Press.
- 30. Sen Gupta, Subrata.Basic Stereochemistry of Organic molecules.
- 31. Kalsi, P. S. Stereochemistry Conformation and Mechanism, Eighth edition, New Age International, 2014.
- 32. Fleming, I. Molecular Orbitals and Organic Chemical reactions, Reference/Student Edition, Wiley, 2009.
- 33. Fleming, I. Pericyclic Reactions, Oxford Chemistry Primer, Oxford University Press.
- 34. Gilchrist, T. L. & Storr, R. C. Organic Reactions and Orbital symmetry, Cambridge University Press.
- 35. Davis, B. G., Fairbanks, A. J., Carbohydrate Chemistry, Oxford Chemistry Primer, Oxford University Press.
- 36. Joule, J. A. Mills, K. Heterocyclic Chemistry, Blackwell Science.
- 37. Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Wiely& Sons (1976).
- 38. Gilchrist, T. L. Heterocyclic Chemistry, 3rd edition, Pearson.
- 39. Bansal, R. K. Heterocyclic Chemistry, New Age International Publishers.
- 40. Davies, D. T., Heterocyclic Chemistry, Oxford Chemistry Primer, Oxford University Press.
- 41. Singh, H. and Kapoor, V. K. Medicinal and Pharmaceutical Chemistry, Vallabh Prakashan, Pitampura, New Delh, 2012.
- 42. Anastas, P.T. & Warner, J.K.: Green Chemistry Theory and Practical, Oxford University Press (1998).
- 43. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
- 44. Cann, M.C. &Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
- 45. Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
- 46. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.
- 47. Ahluwalia, V. K & Kidwai, M. R. New Trends in Green Chemistry, Anamalaya Publishers, 2005.

- 48. R.B. Seymour & C.E. Carraher: Polymer Chemistry: An Introduction, Marcel Dekker, Inc. New York, 1981.
- 49. G. Odian: Principles of Polymerization, 4th Ed. Wiley, 2004.
- 50. F.W. Billmeyer: Textbook of Polymer Science, 2nd Ed. Wiley Interscience, 1971.
- 51. P. Ghosh: Polymer Science & Technology, Tata McGraw-Hill Education, 1991.
- 52. R.W. Lenz: Organic Chemistry of Synthetic High Polymers. Interscience Publishers, New York, 1967.

Physical Chemistry:

- 1. Atkins, P. W. & Paula, J. de Atkins' Physical Chemistry, Oxford University Press
- 2. Castellan, G. W. Physical Chemistry, Narosa
- 3. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press
- 4. Kapoor, K. L. A Textbook of Physical Chemistry, Vol 1-5
- 5. Negi A. S. and Anand, S. C. A Textbook of Physical Chemistry
- 6. Rakshit, P.C., Physical Chemistry, Sarat Book House
- 7. Engel, T. & Reid, P. Physical Chemistry, Pearson
- 8. Levine, I. N. Physical Chemistry, Tata McGraw-Hill
- 9. Maron, S.H., Prutton, C. F., Principles of Physical Chemistry, McMillan
- 10. Ball, D. W. Physical Chemistry, Thomson Press
- 11. Laidler, K. J. Chemical Kinetics, Pearson
- 12. Glasstone, S. & Lewis, G.N. Elements of Physical Chemistry
- 13. Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, Tata-McGraw-Hill
- 14. Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics: Basic Concepts and Methods Wiley
- 15. Moore, W. J. Physical Chemistry, Orient Longman
- 16. Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press
- 17. Atkins, P. W. Molecular Quantum Mechanics, Oxford
- 18. Levine, I. N. Quantum Chemistry, PHI
- 19. Chandra A. K. Introductory Quantum Chemistry
- 20. Prasad R. K. Quantum Chemistry
- 21. Glasstone, S. An Introduction to Electrochemistry, East-West Press
- 22. Barrow, G.M. Physical Chemistry Tata McGraw Hill (2007)
- 23. Banwell, C. N. Fundamentals of Molecular Spectroscopy, Tata-McGraw-Hill
- 24. Barrow, G. M. Molecular Spectroscopy, McGraw-Hill
- 25. Hollas, J.M. Modern Spectroscopy, Wiley India
- 26. McHale, J. L. Molecular Spectroscopy, Pearson Education
- 27. Wayne, C. E. & Wayne, R. P. Photochemistry, OUP
- 28. Rohatgi-Mukherjee, K. K. Fundamentals of Photochemistry
- 29. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3rd Edition
- 30. Brown, J. M. Molecular Spectroscopy, OUP
- 31. McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008)
- 32. Nash, L. K. Elements of Statistical Thermodynamics, Dover
- 33. Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc.
- 34. Seymour, R. B. & Carraher, C. E. Polymer Chemistry: An Introduction, Marcel Dekker, Inc.
- 35. Odian, G. Principles of Polymerization, Wiley
- 36. Billmeyer, F. W. Textbook of Polymer Science, Wiley Interscience, 1971.
- 37. Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005)
- 38. Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007)
- 39. Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5
- 40. Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985)
- 41. Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry Cengage Learning India Pvt. Ltd., New Delhi
- 42. Mahan, B.H. University Chemistry 3rd Ed. Narosa (1998)
- 43. Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985)
- 44. Chugh, K.L., Agnish, S.L. A Text Book of Physical Chemistry Kalyani Publishers
- 45. Bahl, B.S., Bahl, A., Tuli, G.D., Essentials of Physical Chemistry S. Chand & Co. ltd.
- 46. Palit, S. R., Elementary Physical Chemistry Book Syndicate Pvt. Ltd.
- 47. Mandal, A. K. Degree Physical and General Chemistry Sarat Book House
- 48. Pahari, S., Physical Chemistry New Central Book Agency
- 49. Pahari, S., Pahari, D., Problems in Physical Chemistry New Central Book Agency
- 50. Cotton F. A. Chemical Application of Group Theory
- 51. Bishop David M. Group Theory and Chemistry
- 52. Ameta R. Symmetry and Group Theory in Chemistry

<u>Reference Books for Laboratory Experiments</u> Inorganic Chemistry:

- 1. Vogel's Quantitative Chemical Analysis
- 2. Vogel's Qulititative Chemical Analysis
- 3. Spot Tests in Inorganic Analysis F. Feigl & V. Anger
- 4. An Advanced Course in Practical Chemistry Nad, Mahapatra & Ghosal
- 5. Practical Analytical Chemistry, Lab Manual L Kitaw Sintayehu
- 6. Principles of Instrumental Analysis 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
- 7. Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.
- 8. Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5.
- 9. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.

Organic Chemistry:

- 1. Bhattacharyya, R. C, A Manual of Practical Chemistry.
- 2. Vogel, A. I. Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis, CBS Publishers and Distributors.
- 3. Vogel, A. I. Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis, CBS Publishers and Distributors.
- 4. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
- 5. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).
- 6. University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N. University of Calcutta, 2003.
- 7. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- 8. Practical Workbook Chemistry (Honours), UGBS, Chemistry, University of Calcutta, 2015.
- 9. Clarke, H. T., A Handbook of Organic Analysis (Qualitative and Quantitative), Fourth Edition, CBS Publishers and Distributors (2007).
- 10. Arthur, I. V. Quantitative Organic Analysis, Pearson
- 11. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. Green Chemistry Experiment: A monograph, International Publishing House Pvt Ltd. New Delhi. Bangalore CISBN 978-93-81141-55-7, 2013.
- 12. Green Chemistry Monograph, DST Green Chemistry Task Force Committee, New Delhi.

Physical Chemistry:

- 1. Viswanathan, B., Raghavan, P.S. Practical Physical Chemistry Viva Books (2009)
- 2. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson
- 3. Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007)
- 4. Palit, S.R., De, S. K. Practical Physical Chemistry, Science Book Agency
- 5. University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta
- 6. Levitt, B. P. edited Findlay's Practical Physical Chemistry Longman Group Ltd.
- 7. Gurtu, J. N., Kapoor, R., Advanced Experimental Chemistry, S. Chand & Co. Ltd.
- 8. Mukherjee, N.G., Selected Experiments in Physical Chemistry, J. N. Ghose & Sons
- 9. Dutta, S.K., Physical Chemistry Experiments, Bharati Book Stall
- 10. Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
- 11. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- 12. Press W H., Teukolsky S. A., Vellerling W.T. and Flannery B. P. (Eds.), Numerical Recipies in Fortran The art of Scientific Computing; Cambridge Univ. Press (1992).
- 13. Noggle, J. H. Physical chemistry on a Microcomputer, Little Brown & Co. (1985)

Semester -I

Theory Papers

Paper : GE/Chem/TH/01 : (4 Credit, FM-50, 4 L/W; 60L)

Unit : 101G-I : Inorganic Chemistry-I & II (30L):

Inorganic Chemistry-I (15L) :

Atomic Structure (6 L) :

Sommerfeld's Theory. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2 . Quantum numbers and their significances. Radial and angular wave functions. Radial and angular distribution curves. Concept of orbitals and Shapes of *s*, *p*, *d* orbitals.

Acids, Bases and Buffers (4 L):

Arrhenius, Brönsted-Lowry, and Lewis concepts of acids and bases - Factors affecting strengths of acids and bases - Ka, Kb, Kw, pH etc.- Buffers, Henderson's equation - Hydrolysis of salts - Common ion effect.

Chemical Bonding (5 L):

VSEPR theory; Structure of simple molecules and ions of main group elements VB and MO approach of H_2 molecule; MO treatment of homonuclear diatomic molecules (Li₂ to F₂); Concept of HOMO and LUMO.

Inorganic Chemistry-II (15L) :

Coordination Compounds and Transition elements (10 L):

Werner's theory– Nomenclature- Chelates- Stereochemistry of coordination numbers 4, 5 and 6 using hybridizations. Crystal-field theory and crystal-field splitting in octahedral and tetrahedral complexes. CFSE and its calculation in octahedral and tetrahedral - Weak field and strong field- Low spin and high spin complexes.

Chemistry of selected main group elements (5 L):

Hydrogen bonds, Hydrides and dihydrogen - Alkali metal solution in liquid ammonia - Alkali metal anions Complexation of alkali metal ion by crown ether and cryptands, Diborane – structure and bonding - Noble gas compounds.

Unit : 101G-O : Organic Chemistry-I (30L):

1. Fundamentals of Organic Chemistry (2L)

Electronic displacements: inductive effect, resonance and hyperconjugation; cleavage of bonds: homolytic and heterolytic; structure of organic molecules on the basis of VBT; nucleophiles electrophiles; reactive intermediates: carbocations, carbanions and free radicals.

2. Nucleophilic Substitution and Elimination Reactions (2 L)

Nucleophilic substitutions: SN1 and SN2 reactions; eliminations: E1 and E2 reactions (elementary mechanistic aspects); Saytzeff and Hofmann eliminations; elimination vs substitution.

3. Aliphatic Hydrocarbons (11L)

- a) Alkanes: (up to 5 Carbons). Preparation: catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. Reactions: mechanism for free radical substitution: halogenation.
- b) Alkenes: (up to 5 Carbons). Preparation: elimination reactions:

dehydration of alcohols and dehydrohalogenation of alkyl halides; cis alkenes (partial catalytic hydrogenation) and trans alkenes (Birch reduction). Reactions: cis-addition (alkaline KMnO₄) and transaddition (bromine) with mechanism, addition of HX [Markownikoff's (with mechanism) and anti-Markownikoff's addition], hydration, ozonolysis, oxymercuration-demercuration and hydroborationoxidation reaction.

c) Alkynes: (up to 5 Carbons). Preparation: acetylene from CaC₂ and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal dihalides. Reactions: formation of metal acetylides, addition of bromine and alkaline KMnO₄, ozonolysis.

4. Alcohols and ethers (4 L)

- a) Alcohols: (up to 5 Carbons). Preparation: 1°-, 2°- and 3°- alcohols: using Grignard reagent, reduction of aldehydes, ketones, carboxylic acid and esters; Reactions: with sodium, oxidation (alkaline KMnO₄, acidic dichromate, concentrated HNO₃); Oppenauer oxidation;
- b) Diols: Preparation (with OsO₄); pinacol- pinacolone rearrangement with mechanism (with symmetrical diols only).
- c) Ethers: Preparation: Williamson's ether synthesis; Reaction: cleavage of ethers with HI.

5. Aromatic Hydrocarbons (3 L)

Benzene: Preparation: from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions: electrophilic substitution (general mechanism); nitration (with mechanism), halogenations (chlorination and bromination), sulphonation and Friedel-Craft's reaction (alkylation and acylation) (up to 4 carbons on benzene); side chain oxidation of alkyl benzenes (up to 4 carbons on benzene).

6. Amines and diazonium salts (2 L)

- a) Amines: Preparation: Hofmann degradation, by reduction of nitro compounds; Reactions: with HNO₂ (distinction of 1°-, 2°- and 3°- amines), Schotten Baumann reaction.
- b) Diazonium salts: Preparation: from aromatic amines; Reactions: conversion to benzene, phenol, benzoic acid and nitrobenzene, Diazo coupling reaction (with mechanism).

7. Aryl halides (3 L)

Preparation: (chloro-, bromo- and iodobenzene): from phenol, Sandmeyer reactions. Reactions (Chlorobenzene): nucleophilic aromatic substitution (replacement by –OH group) and effect of nitro substituent (activated nucleophilic substitution).

8. Phenols (3 L)

Preparation: cumene hydroperoxide method, from diazonium salts; acidic nature of phenols; Reactions: electrophilic substitution: nitration and halogenations; Reimer-Tiemann reaction, Houben-Hoesch condensation, Schotten-Baumann reaction, Fries rearrangement

LABORATORY EXPERIMENTS

Paper : GE/Chem/PR/01 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 101G-L:</u> Inorganic Chemistry Experiments:

Acid and Base Titrations

- 1. Estimation of carbonate and hydroxide present together in mixture
- 2. Estimation of carbonate and bicarbonate present together in a mixture.
- 3. Estimation of free alkali present in different soaps/detergents.

Oxidation-Reduction Titrations

A. Titration with KMnO₄

- 1. Standardization of $KMnO_4$ solution with standard oxalic acid solution.
- 2. Estimation of Fe(II) using standardized KMnO₄ solution.

B. Titration with K₂Cr₂O₇

- 1. Estimation of Fe(II) using K₂Cr₂O₇ solution.
- 2. Estimation of Fe(III) using $K_2Cr_2O_7$ solution.
- 3. Estimation of Fe(II) and Fe(III) in a given mixture using K₂Cr₂O₇ solution.

Theory Papers :

Paper : GE/Chem/TH/04 : (4 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 404G1-P:</u> Physical Chemistry – I (30L) :

Chemical Kinetics & Catalysis (20L)

Concept of Advancement of reaction, rate, order, rate constant, molecularity, differential & integrated rate equations of different order reactions, experimental methods for determination of order & rate constant of reaction.

Elementary reaction, law of mass action, multistep reactions, rate determining step, steady state approximation and derivation of rate equation, temperature dependence of reaction rates and Arrhenius equation, energy of activation, Arrhenius factor; kinetics of opposing, parallel, consecutive reactions & chain reactions (with examples).

Theories of reaction rates, collision theory and transition state theory (elementary idea)

Catalysis, homogeneous catalysis, acid-base catalysis, enzyme catalysis: Michaelis-Menten equation, turnover number, elementary idea of inhibition, primary kinetic salt effect, and solvent effect (qualitative aspect) of solution phase reactions.

Conductance (10 L)

Ion conductance; Conductance and measurement of conductance, cell constant, conductivity, equivalent conductivity and molar conductivity; Variation of conductivity and equivalent conductivity with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductivity at infinite dilution and their determination for strong and weak electrolytes.

Unit : 404G2-O: Organic Chemistry –II (15L)

1. Stereochemistry (4 L):

Different types of isomerism; geometrical and optical isomerism; concept of chirality and optical activity (up to two carbon atoms); asymmetric carbon atom; elements of symmetry (plane and centre); interconversion of Fischer and Newman representations; enantiomerism and diastereomerism, meso compounds; threo and erythro, D and L, cis and trans nomenclature; CIP Rules: R/S (upto 2 chiral carbon atoms) and E/Z nomenclature.

2. Carbonyl Compounds (7 L) :

Aldehydes and Ketones (aliphatic and aromatic): (Formaldehye, acetaldehyde, acetone and benzaldehyde): Preparation: from acid chlorides, from nitriles and from Grignard reagents; general properties of aldehydes and ketones; Reactions: with HCN, ROH, NaHSO₃, NH₂-G derivatives and with Tollens' and Fehling's reagents; iodoform test; aldol condensation (with mechanism); Cannizzaro reaction (with mechanism), Wittig reaction, benzoin condensation; Clemmensen reduction, Wolff-Kishner reduction and Meerwein-Pondorff- Verley (MPV) reduction.

3. Carboxylic acid and derivatives (4L):

- a. Carboxylic acids (aliphatic and aromatic): strength of organic acids: comparative study with emphasis on factors affecting pK values; Preparation: acidic and alkaline hydrolysis of esters (BAc2 and AAC2 mechanisms only) and from Grignard reagents; Reactions: Hell Vohlard Zelinsky reaction and Claisen condensation; Perkin reaction.
- b. Carboxylic acid derivatives (aliphatic): (up to 5 carbons). Preparation and reactions of acid chlorides, anhydrides, esters and amides, Reformatsky reaction.

Unit: 404G2-P: Physical Chemistry – II (15L)

Photophysics & photochemistry :

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, absorption, molar extinction coefficient and its physical significance. Franck Condon principle, Luminescence: resonance radiation, fluorescence,

phosphorescence & chemiluminescence, Jablonski diagram, singlet and triplet states, decays of excited states by radiative and non-radiative pathways, internal conversion (IC) and intersystem crossing (ISC); Laws of photochemistry, quantum yield, photosensitized reactions, photostationary state.

Laboratory Experiments :

Paper : GE/Chem/PR/04 : (2 Credit, FM-50, 4 L/W; 60L)

<u>Unit : 404G-L :</u> Organic Chemistry and Physical Chemistry Laboratory Experiments:

Organic Chemistry (30 L) :

- A. Qualitative Analysis of Single Solid Organic Compound(s)
- 1. Detection of special elements (N, Cl, and S) in organic compounds.
- 2. Solubility and Classification (solvents: H₂O, dil. HCl, dil. NaOH).
- 3. Detection of functional groups: Aromatic-NO₂, Aromatic -NH₂, -COOH, carbonyl (no distinction of -CHO and >C=O needed), -OH (phenolic) in solid organic compounds.

(Experiments 1 to 3 with unknown (at least 4) solid samples containing not more than two of the above type of functional groups should be done.)

B. Identification of a pure organic compound (at least three from the list)

- 1. Solid compounds: oxalic acid, tartaric acid, succinic acid, resorcinol, urea, glucose, benzoic acid and salicylic acid.
- 2. Liquid Compounds: methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene.

Physical Chemistry (30 L) :

- 1. Determination of the surface tension of supplied solutions by drop weighing method.
- 2. Determination of the distribution coefficient of iodine between non aqueous and aqueous solvents.
- 3. Determination of rate constants of acid catalyzed hydrolysis methyl acetate at two acid concentrations.
- 4. Determination of the viscosity coefficient of supplied liquid using Ostwald Viscometer.
- 5. Study and draw the phase diagram of ternary system of water, benzene and glacial acetic acid.

Reference Books (Theory):

Inorganic Chemistry:

General and Inorganic Chemistry (Volume I & II) – R. P. Sarkar.

Organic Chemistry:

- 1. Bahl, A. & Bahl, B.S. Advanced Organic Chemistry, S. Chand, 2010.
- 2. Sen Gupta, S. Organic Chemistry, Oxford University Press, 2014.

Physical Chemistry:

- 1. Atkins, P. W. & Paula, J. de Atkins' Physical Chemistry, Oxford University Press.
- 2. Castellan, G. W. Physical Chemistry, Narosa.
- 3. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press.
- 4. Laidler, K. J. Chemical Kinetics, Pearson.
- 5. Barrow, G.M. Physical Chemistry Tata McGraw-Hill (2007).
- 6. Banwell, C. N. Fundamentals of Molecular Spectroscopy, Tata-McGraw-Hill.
- 7. Barrow, G. M. Molecular Spectroscopy, McGraw-Hill.

Reference Books for Laboratory Experiments:

Inorganic Chemoistry :

1. An Advanced Course in Practical Chemistry - Nad, Mahapatra & Ghosal.

Organic Chemistry :

- 1. University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta, 2003.
- 2. Bhattacharyya, R. C, A Manual of Practical Chemistry.

Physical Chemistry :

- 1. Mukherjee, N.G., Selected Experiments in Physical Chemistry J. N. Ghose & Sons.
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