Syllabus

Five Year Integrated M.Sc. Program in Chemistry

(under CBCS, *w.e.f.* Academic Session 2018-2019)

Offered By

Department of Chemistry and Chemical Sciences

CENTRAL UNIVERSITY OF JAMMU
Rahya-Suchani (Bagla), District-Samba
Jammu-181143, (J&K) India

General Note for Paper Setting

- The Question Papers for the Mid-Semester Examination shall be as follows:

1. In four credit course, the paper shall be of 2 (two) hours duration and shall comprise the following sections:

Section	Type	No. of Questions	To Attempt	Marks per question	Marks
A	Objective	10	10	1	10
B	Short Answer Type	5	3	6	18
C	Essay/Long Answer Type	2 (with internal choice)	2	11	22
Total					**50**

a. **Section A** shall have 10 (Ten) Objective Type Questions (Multiple choices) of one mark each. All questions in this section shall be compulsory (Total 10 Marks).
b. **Section B** shall have 5 (Five) Short Answer Questions (SAQ) of 6 (six) Marks each, out of which the examinees shall be required to attempt any three questions (Total 18 Marks).
c. **Section C** shall have 2 (Two) Essay/Long Answer Questions (one from each unit with internal choice), of 11 (Eleven) Marks each (Total 22 Marks); alternatively, if the course so requires, this section may comprise a case study of 11 marks and one question with internal choice of 11 Marks.

- The Question Papers for the End-Semester Examination shall be as follows:

2. In four credit course, the paper shall be of 3 (three) hours duration and shall comprise the following sections:

Section	Type	No. of Questions	To Attempt	Marks per question	Marks
A	Objective	10	10	1.5	15
B	Short Answer Type	10 (with internal choice)	5	8	40
C	Essay/Long Answer Type	5	3	15	45
Total					**50**

a. **Section A** shall have 10 (Ten) Objective Type Questions (Multiple choice), two from each unit. Each question shall be of 1.5 marks *(Total 15 marks).* All questions in this section shall be compulsory.
b. **Section B** shall have 10 (Ten) Short Answer Questions, two from each unit. Each question shall be of 8 (Eight) marks. The candidate is required to attempt any five questions selecting one from each unit *(Total 40 marks).*
c. **Section C** shall have 5 (Five) Essay/Long Answer Questions, one from each unit. Each question shall be of 15 (fifteen) marks. The candidate is required to attempt any three questions (Total 45 marks).

Course Matrix for Five Year Integrated M.Sc. Chemistry

Semester	Core		DSE		ID		F	Total
	Theory	Lab	Theory	Lab	Theory	Lab		
I	8	4	-	-	4	4	4	24
II	8	4	-	-	8	4	4	28
III	12	6	-	-	4	-	4	26
IV	12	4	-	4	-	-	4	24
V	8	5	8	3	-	-	-	24
VI	8	6	8	-	-	-	-	22
VII	8	8	4	-	-	-	4	24
VIII	8	6	4	-	-	-	4	22
IX	8	10	4	-	4	-	-	26
X	-	12	4	-	4	-	-	20
Total								240

Semesters I to VI: 148 Credits
Semesters VII to X: 92 Credits

Course Type	Code
Departmental Core Course	C
Discipline Specific Elective	DSE
Interdisciplinary	ID
Foundation	F

Semester - I

Course Code	Course	Type	Credits	Contact hours per week (L-T-P)
	General Chemistry-I	C	4	3-1-0
	General Chemistry Lab-I	C	4	0-0-8
	Mathematics-I	C	4	3-1-0
	Botany-I		4	3-1-0
	Zoology-I		4	3-1-0
	Physics-I	IDC	4	3-1-0
	Physics Lab-I	IDC	4	0-0-8
	English	F	4	3-1-0
	Total		24	

Semester – II

Course Code	Course	Type	Credits	Contact hours per week (L-T-P)
	General Chemistry-II	C	4	3-1-0
	General Chemistry Lab-II	C	4	0-0-8
	Mathematics-II	C	4	3-1-0
	Botany-II		4	3-1-0
	Zoology-II		4	3-1-0
	Physics-II	IDC	4	3-1-0
	Physics Lab-II	IDC	4	0-0-8
	Environmental Science	IDC	4	3-1-0
	Introduction to Computers	F	4	3-1-0
	Total		28	

Semester – III

Course Code	Course	Type	Credits	Contact hours per week (L-T-P)
	Inorganic Chemistry-I	C	4	3-1-0
	Organic Chemistry-I	C	4	3-1-0
	Physical Chemistry-I	C	4	3-1-0
	Inorganic Chemistry Lab-I	C	3	0-0-6
	Organic Chemistry Lab-I	C	3	0-0-6
	Biochemistry	IDC	4	3-1-0
	Communication Skills	F	4	3-1-0
	Total		26	

Semester – IV

Course Code	Course	Type	Credits	Contact hours per week (L-T-P)
	Inorganic Chemistry-II	C	4	3-1-0
	Organic Chemistry-II	C	4	3-1-0
	Physical Chemistry-II	C	4	3-1-0
	Organic Chemistry Lab-II	C	4	0-0-8
	Physical Chemistry Lab-I	DSE	4	0-0-8
	Basic Analytical Chemistry	F	4	3-1-0
	Total		24	

Semester – V

Course Code	Course	Type	Credits	Contact hours per week (L-T-P)
	Organic Spectroscopy and Compounds with Heteroatoms	C	4	3-1-0
	Quantum Mechanics, Surface and Colloidal Chemistry	C	4	3-1-0
	Seminar	C	2	0-0-4
	Physical Chemistry Lab-II	C	3	0-0-6
	Properties of Inorganic Metal Complexes	DSE	4	3-1-0
	Natural Products Chemistry	DSE	4	3-1-0
	Inorganic Chemistry Lab-II	DSE	3	0-0-6
	Total		24	

Semester – VI

Course Code	Course	Type	Credits	Contact hours per week (L-T-P)
	Selected Topics in Inorganic Chemistry	C	4	3-1-0
	Bioorganic and Heterocyclic Chemistry	C	4	3-1-0
	Project/Dissertation	C	6	0-0-12
	Spectroscopy and Computational Chemistry	DSE	4	3-1-0
	Applied Chemistry	DSE	4	3-1-0
	Total		22	

Semester – VII

Course Code	Course	Type	Credits	Contact hours per week L-T-P
	Bonding Theories and Inorganic Reaction Mechanisms	C	4	3-1-0
	Organic Reaction Mechanism and Stereochemistry	C	4	3-1-0
	Preparation of Inorganic Complexes and Analysis Lab	C	3	0-0-6
	Organic Preparation and Qualitative Analysis Lab	C	3	0-0-6
	Seminar	C	2	0-0-4
	Quantum Chemistry and Chemical Dynamics	DSE	4	3-1-0
	Analytical Chemistry	F	4	3-1-0
	Total		24	

Semester – VIII

Course Code	Course	Type	Credits	Contact hours per week L-T-P
	Group Theory, Transition Metal Chemistry and Photochemistry	C	4	3-1-0
	Group Theory and Spectroscopy	C	4	3-1-0
	Organic Synthesis and Chromatography Lab	C	3	0-0-6
	Thermodynamic, Kinetics and Spectroscopy Lab	C	3	0-0-6
	Organic Synthesis and Reaction Mechanism	DSE	4	3-1-0
	Organic Spectroscopy and Organometallics	F	4	3-1-0
	Total		22	

Semester – IX

Course Code	Course	Type	Credits	Contact hours per week L-T-P
	Thermodynamics and Electrochemistry	C	4	3-1-0
	Reagents, Photochemistry and Heterocyclic Chemistry	C	4	3-1-0
	Inorganic Preparation, Analysis and Chromatography Lab	C	3	0-0-6
	Electrochemistry and Computational Chemistry Lab	C	3	0-0-6
	Project Phase I	C	4	0-0-8
	Bio-inorganic and Supramolecular Chemistry	DSE	4	3-1-0
	Selected Topics in Physical and Inorganic Chemistry	ID	4	3-1-0
	Total		26	

Semester – X

Course Code	Course	Type	Credits	Contact hours per week L-T-P
	Project/Dissertation	C	12	0-0-24
	Green Chemistry (or) Computational Chemistry (or) Organometallic Chemistry (or) Solid State Chemistry	DSE	4	3-1-0
	Nano Chemistry	ID	4	3-1-0
	Total		20	

Semester: I
Course Name: General Chemistry-I
Course Code: **4 Credits (3-1-0)**

UNIT – I **14 hours**

Atomic structure and wave mechanics: Characteristics of Black-body radiation, Planck's radiation law, Photoelectric effect, Compton effect, Bohr's model of hydrogen atom and its limitations. Rutherford's atomic model, Bohr's theory, Dual nature of electrons, de Broglie hypothesis and its derivation, Heisenberg's uncertainty principle, Schrodinger wave equation and its importance, Physical interpretation of the wave function, Significance of Ψ and Ψ^2, Radial and angular wave functions, Probability distribution curves.

Quantum numbers and their significance, Atomic orbitals, Shapes of *s*, *p*, *d* orbitals and their characteristics, Aufbau and Pauli exclusion principles, Hund's multiplicity rule and (n+l) rule, Electronic configurations of the elements (*s*, *p* and 3*d*-block elements), Effective nuclear charge, Slaters' rule with some exercises.

UNIT – II **10 hours**

Periodic table and periodicity of properties: Long form of periodic table, Classification of elements as main group, transition and inner transition elements, Periodicity in the following properties: Atomic radius, Covalent, Ionic and van der Waals radii, Ionization energy, Electron affinity, Electronegativity: Definition, Methods of determination-Pauling's, Mulliken's and Allred-Rochow's scales, Numerical problems, Inert pair effect.

UNIT – III **12 hours**

Basics of organic chemistry: Classification and nomenclature of organic compounds, Hybridization, Shapes of molecules, Influence of hybridization on bond lengths, Bond angles and bond energy, Inductive effect, Polar covalent bonds and dipole moment, Delocalized bonds and resonance, Drawing resonance structures, Concept of formal charge, Hyperconjugation, Steric effect, Steric inhibition of resonance, Hydrogen bonding, Inter- and intramolecular hydrogen bonding, Effect on boiling point and solubility.

UNIT – IV **12 hours**

Introduction to types of organic reactions and their mechanism: Addition, elimination, substitution and rearrangement reactions, Homolytic and heterolytic C–C bond fission, Electrophiles and nucleophiles, Structure and stability of reactive intermediates: carbocations, carbanions and free radicals.

Aromaticity: Resonance in benzene, Huckel's rule, Aromatic, non-aromatic and anti-aromatic compounds, Aromatic character of arenes, Cyclic carbocations/carbanions and heterocyclic compounds with suitable examples, Electrophilic substitution reactions in aromatic compounds, General mechanisms of nitration, halogenation, sulphonation, Friedel-Craft's acylation and alkylation, *ortho*/*para*/*meta* directive effect of substituents.

UNIT – V **12 hours**

Stereochemistry: Concept of isomerism, Optical isomerism, Chirality and elements of symmetry, Classification of stereoisomers, Enantiomersim and diasteroisomerism involving one and two chiral centers, *Meso*/*dl* and *erythro*/*threo* isomers, Relative and absolute configurations, *D-L*, *R-S* systems of nomenclature, Fischer, Newmann and Sawhorse projection formulae and their interconversion, Conformational analysis of ethane and *n*-butane, Geometrical isomerism: *cis-trans syn-anti*, *E-Z* notations, Geometrical isomerism in oximes, cumulenes and alicyclic compounds.

REFERENCES

1. J. D. Lee, *Concise Inorganic Chemistry*, 5th Ed., Wiley, 2008.
2. K. M. Mackay and R. A Mackay, *Introduction to Modern Inorganic Chemistry*, 4th Ed., Nelson Thornes*,* 1990.
3. B. R. Puri, L. R. Sharma and K. C. Kalia, *Principles of Inorganic Chemistry*, Vishal Publishing, 2017.
4. F. A. Cotton and G. Wilkinson, C. A. Murillo and M. Bochmann, *Basic Inorganic Chemistry*, 6th Ed., John Wiley, 1999.
5. J. E. Huheey, Harpes and Row, *Inorganic Chemistry*, 4th Ed., 2006.
6. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Ed., Pearson, 2018.
7. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Ed., 2010.
8. A. Bahl and B. S. Bahl, *Advanced Organic Chemistry*, 21st Ed., 2012.
9. T. W. Graham Solomons, *Fundamentals of Organic Chemistry*, John Wilev, 5th Ed., 1998.
10. Streitwiesser, Hathcock and Kosover, *Introduction to Organic Chemistry*, Macmillan, 4th Ed., 1992.
11. L.G. Wade Jr., *Organic Chemistry*, Prentice Hall, 8th Ed., 2012.
12. P. Y. Bruice, *Organic Chemistry*, 7th Ed., 2012.

Semester: I
Course Name: General Chemistry Lab-I
Course Code: **4 Credits (0-0-8)**

General Instructions: Demonstration and concept of good lab practices including safety, chemical/glassware handling, chemical nature understanding, waste management, notebook maintenance.

Part A
1. Calibration and use of apparatus
2. Preparation of solutions of different Molarity/Normality

Part B: Volumetric Analysis (Any 8 Experiments):
Acid-Base Titrations
1. Titration of HCl Vs NaOH (strong acid Vs strong base)
2. Titration of HCl Vs Na_2CO_3 (strong acid Vs weak base)
3. Titration of Oxalic acid Vs NaOH (weak acid Vs strong base)
4. Titration of Acetic acid (commercial vinegar) Vs NaOH (weak acid Vs strong base)

Permanganometry
1. Estimation of ferrous and ferric ions in a mixture
2. Estimation of oxalic acid
3. Estimation of calcium (Chalk)

Dichrometry
1. Determination of the percentage purity of the given sample of $FeSO_4(NH_4)_2SO_4.6H_2O$ [Mohr's salt]
2. Standardization of sodium thiosulphate using potassium dichromate and estimation of iodine

Part C: Purification of organic compounds by crystallization (At least four compounds)
Compounds: Phthalic acid, Acetanilide, Naphthalene, Benzoic acid etc.
Solvents: Water, Ethanol, Aqueous ethanol

Part D: Determination of melting point
Determination of meting point of at least four organic compounds.

REFERENCES:

1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny *Vogel's Text book of Quantitative Chemical Analaysis*, 5/e., LBS.
2. V. K. Ahluwalia, S. Dhingra and A. Gulate, *College Practical Chemistry.*, 2008 (reprint), Universities Press (India) Pvt Ltd.
3. O. P. Pandey, D. N. Bajpai and S. Giri, *Practical Chemistry, for I, II & III BSc. Students,* 2009 (reprint), S. Chand & Company Ltd.
4. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, *Basic Principles of Practical Chemistry*, 2004, Sultan Chand and Sons, New Delhi.
5. In-house laboratory manual with experimental procedures and relevant information

Semester: II
Course Name: General Chemistry-II
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Chemical bonding-I: Covalent Bond, Valence bond theory and its limitations, Directional characteristics of covalent bond, Various types of hybridization and Shapes of simple inorganic molecules and ions, Valence shell electron pair repulsion (VSEPR) theory to NH_3, H_3O^+, SF_4, ClF_3, ICl_2, and H_2O, Molecular orbital theory, Postulates, Criteria for forming MO, Construction of MO's by LCAO, Physical picture of bonding and antibonding wave functions, Concept of σ, σ*, π, π* orbitals and their characteristics, Discussion about homonuclear (He_2, N_2, O_2, F_2, C_2) and Heteronuclear (CO and NO) diatomic molecules, Bond order and bond energy, Calculation of percentage ionic character from dipole moment and electronegativity difference, Comparison of MO and VB theories, Basic concept of resonance.

UNIT – II **12 hours**

Chemical bonding-II: Properties of ionic compounds, Unit cell, Types of unit cells, Packing in ionic solids, Structures of some common ionic solids, AB-type: NaCl, ZnS-zinc blende and wurtzite, CsCl, AB_2-type: CaF_2, A_2B-type: Na_2O, Radius ratio effect and Coordination number, Limitation of radius ratio rule, Lattice defects, Semiconductors, Lattice energy and Born-Haber cycle, Solvation energy and solubility of ionic solids, Polarizing power and polarisability of ions, Fajan's rule, Metallic bonding: Qualitative idea of free electron, Valence bond and Band theories, Conducting, Semi conducting and Insulating properties, Weak interactions, Hydrogen bonding, van der Waals forces.

UNIT – III **12 hours**

Gaseous state of matter: Postulates of kinetic theory of gases, Gas laws from kinetic equation, Relation between kinetic energy and temperature, Thermal motion of molecules, Maxwell distribution of molecular velocities and kinetic energies, Effect of temperature, Most probable velocity, Average velocity and root mean square velocity, Evaluation of these velocities using Maxwell equation.

Collision theory, Collision diameter, Collision cross section, Collision number, Collision frequency and mean free path, Degrees of freedom of gaseous molecule: Translational, rotational and vibrational.

Deviation from ideal behavior, Equation of state for real gases (van der Waals equation), Virial equation of state, Critical phenomenon, Critical constants, Law of corresponding states.

UNIT – IV **12 hours**

Thermodynamics-I: Thermodynamic terms, State functions, path functions and their differentials, Thermodynamic process, Concept of heat and work, First Law of thermodynamics, Internal energy and enthalpy, Heat capacity, Heat capacities at constant volume and pressure and their relationship, Joule's law, Joule–Thomson experiment, Joule–Thomson coefficient and inversion temperature, Calculation of w, q, dU & dH for the expansion of ideal gases under isothermal and adiabatic condition for reversible process, Zeroth law of thermodynamics.

Thermochemistry: Hess's law of constant heat summation, Exothermic and endothermic reactions, Standard enthalpy changes, Types of enthalpy changes: formation, combustion, neutralization, Kirchhoff's equation, Bond energy, Numericals.

UNIT – V **12 hours**

Thermodynamics-II: Second law of thermodynamics, Heat engine, Carnot cycle and its efficiency, Concept of entropy, Physical significance of entropy, Entropy change in an ideal gas, Entropy as a function of temperature, volume and pressure, Entropy change of universe, Combined statement of first and second laws of thermodynamics, Entropy change for isolated systems, Thermodynamic relations based on 2nd law: energy as a function of temperature and volume, enthalpy as a function of temperature and pressure.

REFERENCES

1. B. R. Puri, L. R. Sharma and K. K. Kalia, *Principles of Inorganic Chemistry*, 23rd Ed., New Delhi, Shoban Lal Nagin Chand & Co, 1993.
2. J. D. Lee, *Concise Inorganic Chemistry*, 5th Ed., UK, John Wiley & Sons, 2006 .
3. K. M. Mackay and R. A Mackay, *Introduction to Modern Inorganic Chemistry*, 4th Ed., Nelson Thornes*,* 1990.
4. G. Wilkinson, R. D. Gillars and J. A. Mccleverty, *Comprehensive Coordination Chemistry,* Pergamon, 1987.
5. N. N. Greenwood and Earnshow, *Chemistry of the Elements*, 2nd Ed., Pergamon, 1997.
6. P. W. Atkins, *The Elements of Physical Chemistry*, Oxford, 10th Ed., 2016.
7. R. P. Rastogi and R. R. Mishra, *Chemical Thermodynamics*, Vikas Publishing House Pvt. Ltd., 6th Ed., 2009.
8. K. L. Kapoor, *A Text Book of Physical Chemistry*, McGraw Hill Education (India) Pvt. Ltd., Vol. 3, 5th Ed., 2014.
9. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Co., 47th Ed., 2017.

Semester: II
Course Name: General Chemistry Lab-II
Course Code: **4 Credits (0-0-8)**

Part A: Qualitative inorganic analysis (At least six mixtures)

Qualitative semi-micro analysis of mixtures containing two anions

List of anions: CO_3^{2-}, S^{2-}, SO_4^{2-}, NO_3^-, NO_2^-, $(CO_2)_2^{2-}$, F^-, Cl^-, Br^-, I^-, SCN^-, $S_2O_3^{2-}$, BO_3^{3-} etc.

Part B: Technical analysis (At least six experiments)

1. Estimation of iodine in antiseptic drug through drug analysis
2. Estimation of available chlorine in the given bleaching powder sample
3. Estimation of manganese dioxide in pyrolusite
4. Determination of CaO in the given sample of commercial lime
5. Estimation of nitrogen in a given fertilizer (inorganic)
6. Determination of iodine value of an oil sample
7. Determination of saponification value of an oil sample

REFERENCES:

1. V. V. Ramanujam, *Inorganic Semi Micro Qualitative Analysis*, 3rd Ed., 1974, National Publishing Company, Chennai.
2. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, *Vogel's Text Book of Inorganic Qualitative Analysis*, 4th Ed., 1974, ELBS, London.
3. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, *Basic Principles of Practical Chemistry*, 2nd Ed., 2004, Sultan Chand and Sons, New Delhi.
4. In-house laboratory manual with experimental procedures and relevant information.

Semester: III
Course Name: Inorganic Chemistry-I
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Chemistry of *s*-block elements: General characteristics and comparative study of *s*-block elements, Position of hydrogen in the periodic table, Atomic hydrogen, Nascent hydrogen, Uses of hydrogen, Diagonal relationships, Salient features of hydrides, Solvation and complexation tendencies including their function in biosystems, An introduction to alkyls and aryls.

Chemistry of noble gases: Chemical properties of the noble gases, Chemistry of xenon, Structure and bonding in xenon compounds (oxides and fluorides: XeF_4, XeF_6, XeO_3 and $XeOF_4$), Uses of noble gases.

UNIT – II **12 hours**

Chemistry of *p*-block elements: General characteristics of *p*-block elements and their compounds, Comparative study (including diagonal relationships) of groups 13-17 elements with reference to electronic configuration, Atomic radii and ionic radii, Oxidation states, Ionisation enthalpy, Electron affinity, Electronegativity.

Chemistry of group 13 elements: Chemistry of boron, Boron hydrides (preparation, structure, bonding, reactions and properties) Wade's rule, Boron halides, Boron-nitrogen chemistry, Boron-oxygen chemistry, Borane, Carborane and metalloborane.

Chemistry of group 14 elements: Allotropes of carbon: Diamond, Graphite and Fullerenes, Intercalation compounds, Carbides, Carbon halides and oxides, Compounds with C–N and C–S bonds, Silane reagents, Synthesis, Properties and modifications on polysilanes, Silicides, Silicone polymers, Oxygen compounds of silicon.

UNIT – III **12 hours**

Chemistry of group 15 elements: Nitrides, Hydrides of nitrogen, Oxides of nitrogen, Oxo acids and anions of nitrogen, Activation of nitrogen, Reaction of coordinated NO, Phosphides, Phosphorous halides and oxides, Oxoacids of phosphorous and their salts.

Chemistry of group 16 elements: Paramagnetic nature of oxygen, Preparation, Properties, Structure and uses of oxyacids of sulphur, Classification of oxides based on their chemical behaviour–Acidic oxide, Amphoteric oxide and neutral oxides, Peroxides, Super oxides, Dioxides, Sub oxides and mixed oxides.

Chemistry of group 17 elements: Peculiarities of fluorine, Hydrides, Oxides and oxo acids of halogens, Inter halogen compounds and pseudo halogens.

UNIT – IV **12 hours**

Coordination chemistry-I: Double salts, Complex compounds, Complex ion and coordination number, Ligands and their classification, Chelates and their uses, IUPAC nomenclature of coordination compounds, Isomerism (structural and geometrical), Valence bond theory and its applications to transition metal complexes (outer and inner orbital complexes), Limitations of valence bond theory, Werner's Coordination theory and its experimental verification, Effective atomic number.

UNIT – V **12 hours**

Coordination chemistry-II: Metal-ligand bonding in transition metal complexes-An elementary idea of crystal field theory, Crystal field splitting in octahedral, tetrahedral and square planar complexes, Factors affecting the crystal-field parameters, Crystal field stabilization energy (CFSE), Spectrochemical series, Measurement of (10 Dq or Δo) in weak field and strong field complexes, Pairing energy, Effects of CFSE on hydration energy, Electroneutrality principle.

Thermodynamic and kinetic aspects of metal complexes: Stability of coordination compounds – Stability constants, Stepwise formation constants, Overall formation constants, Relationship between stepwise and overall formation constants, Difference between thermodynamic and kinetic stability, Determination of stability constants by: Spectrophotometric methods (Job's method, Mole ratio and slope ratio method), Bjerrum's method, Leden's method and Polarographic method.

REFERENCES

1. J. D. Lee, *Concise Inorganic Chemistry*, 5th Ed., Chapman & Hall, London, 1996.
2. B. R. Puri, L. R. Sharma and K. C. Kalia, *Principles of Inorganic Chemistry*, Shoban Lal Nagin Chand & Co., New Delhi, 2001.
3. P. L. Soni, *Text Book of Inorganic Chemistry*, Sultan Chand & Sons, New Delhi, 1993.
4. Malik, Tuli and Madan, *Selected Topics in Inorganic Chemistry*, S. Chand & company, New Delhi, 2002.
5. J. E. Huheey, E. A. Keiter, R. L .Keiter and O. K. Medhi, *Principles of Structure and Reactivity*, 1st Ed., Pearson Education, 2006.
6. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, Oxford University Press, 2006.
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9. G. Wulfsberg, *Inorganic Chemistry*, 2nd Ed., Viva Publisher, 2005.
10. F. A Cotton, G. Wilkinson and P. L. Gaus, *Basic Inorganic Chemistry*, 3rd Ed., John Wiley & Sons, New York, 1995.
11. H. J. Arnikar, *The Essential Theories of Nuclear Chemistry*, 4th Ed., New Age International, 1995.
12. K. J. Laidller, *Chemical Kinetics*, 3rd Ed., Pearson, 2003.
13. S. H. Maron and C. F. Prutton, *Principles of Physical Chemistry*, 4th Ed., Collier Macmillan, 1965.
14. S. Glasstone and D. Lewis, *Elements of Physical Chemistry*, 2nd Ed., Palgrave Macmillan, 1963.
15. P. Atkins and J. D. Paula, *Physical Chemistry*, 10th Ed., 2014.

Semester: III
Course Name: Organic Chemistry-I
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Alkanes: Nomenclature, Formation of alkanes, Corey House reactions, Decarboxylation of carboxylic acids, Wurtz Reaction, Wurtz-Fittig Reaction, Free-radical halogenation of alkanes.

Cycloalkanes: Nomenclature, Methods of preparations, Types of cycloalkanes and their relative stability, Bayer's strain theory and its limitations, Ring strain in cyclopropane and cyclobutanes, Ring inversion of cyclohexane with energy diagrams, Relative stability of chair, boat and twist boat forms.

UNIT – II 12 hours

Alkenes: Nomenclature of alkenes, Formation of alkenes by elimination reactions: Dehydration, dehydrohalogenation and dehalogenation, Mechanisms of E1, E2, E1cB reactions, Regioselectivity, Saytzeff rule, Hoffmann elimination, Reactions of alkenes, Electrophilic additions and their mechanisms (Markovnikov/Anti-Markovnikov addition), Mechanism of oxymercuration-demercuration, hydroboration-oxidation, Epoxidation, Ozonolysis, Hydrogenation, *syn*- and *anti*-Hydroxylation, Polymerization.

UNIT – III 12 hours

Dienes and Cycloalkenes: Nomenclature and classification of dienes: Isolated, conjugated and cumulated dienes, Structure of allenes and butadiene, Methods of formation, Polymerization, 1,2- and 1,4-addition reactions of conjugated dienes, Diels-Alder reaction, Methods of formation and chemical reactions of cycloalkenes.

Alkynes: Nomenclature, Structure and bonding in alkynes, Methods of formation, Acidity of alkynes, Chemical reactions of alkynes, Mechanism of electrophilic and nucleophilic addition reactions, Hydration to form carbonyl compounds, Hydroboration-oxidation, Metal-ammonia reductions, Oxidation and polymerization.

UNIT – IV 12 hours

Carbonyl compounds I: Nomenclature, Structure of the carbonyl group, Synthesis of aldehydes and ketones: Oxidation of alcohols, Oppenauer oxidation, Synthesis from acid chlorides, Rosenmund reduction, Friedel-Crafts reaction, Synthesis of aldehydes and ketones using 1,3-dithianes, Synthesis of ketones from nitriles and from carboxylic acids, Physical properties, Nucleophilic addition to carbonyl group, Mechanism of Aldol, Benzoin and Knoevenagel condensations, Perkin, Cannizzaro, Claisen-Schmidt, Wittig reactions, Baeyer-Villiger oxidation, Benzil-Benzilic acid and Beckmann rearrangements, MPV, Clemmensen, Wolff-Kishner, $LiAlH_4$ and $NaBH_4$ reductions, Halogenation of enolizable ketones, α-Substitution reactions, Use of acetal as protecting group, Introduction to α,β-unsaturated carbonyl compounds, Michael addition.

UNIT – V 12 hours

Carbonyl compounds II: Active methylene compounds: Acidity of α-hydrogens, Keto-enol tautomerism, Preparation of ethyl acetoacetate, Alkylation of diethyl malonate and ethyl acetoacetate, Synthetic applications of ethyl acetoacetate: Synthesis of ketones, Carboxylic acids and Ketonic acids, Biginelli reaction, Hantszch dihydropyridine synthesis, Synthetic applications malonic ester: Synthesis of disubstituted acetic acid, α-Substituted succinic acids, Ketones and Ketonic acids.

REFERENCES

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7^{th} Ed., 2010.
2. T. W. Graham Solomons, *Fundamentals of Organic Chemistry*, John Wiley, 5^{th} Edition, 1998.
3. Streitwiesser, Hathcock and Kosover, *Introduction to Organic Chemistry*, Macmillan, 4^{th} Ed., 1992.
4. I. L. Finar, *Organic Chemistry*, Vol. I and II, 6^{th} Ed., 2002.
5. P. Sykes, *A Guide Book to Mechanism in Organic Chemistry*, 6^{th} Ed., 2003.
6. S. H. Pine, *Organic Chemistry*, 5^{th} Ed., 2007.
7. M. B. Smith, *March's Advanced Organic Chemistry, Reactions, Mechanisms and Structure*, 7^{th} Ed., 2016.
8. L.G. Wade Jr., *Organic Chemistry*, Prentice Hall, 8^{th} Ed., 2012.
9. P. Y. Bruice, *Organic Chemistry*, 7^{th} Ed., 2012.
10. P. S. Kalsi, *Organic Reactions and their Mechanisms*, 4^{th} Ed., New Age International, 2017.

Semester: III
Course Name: Physical Chemistry I
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Mathematical functions: Idea of algebraic and transcendental functions, Complex number, Trigonometric, logarithmic and exponential functions, Simple problems, Graphical representation of functions, Cartesian Coordinate system, Rules for drawing graph from the data of chemical properties, Equation of straight line, slope and intercept.

Differentiation: Basic concepts, Continuity, Limit, Differentiation by rule, Exact and inexact differentials, Logarithmic differentiation, Successive differentiation, Stationary point, Evaluation of maxima and minima, Partial differentiation, Simple problems.

UNIT – II **12 hours**

Integration: Basic concepts, Indefinite integral: differential and integral operators, Integration by parts, Definite integral: properties of the definite integral, Infinite integrals, Even and odd functions, Basic idea of double integral, Volume integral and standard integrals, Average value, Simple problems.

Differential equations: First order differential equation, Analytical solution of differential equation, Separable equations, First-order linear equations, The general solution: two distinct real roots, A real double root, Complex roots and particular solutions using initial and boundary conditions, Second order differential equation with constant coefficients, Homogeneous linear equations (only $y'' + ay' + by = 0$ and $y'' + k^2y = 0$ type), Simple problems.

UNIT – III **12 hours**

Thermodynamics-III: Third law, Nernst Heat theorem, Statement and concept of residual entropy, Evaluation of absolute entropy from heat capacity data, Gibbs and Helmholtz functions, *G* and *A* functions as thermodynamic quantities, *A* and *G* as criteria for thermodynamic equilibrium and spontaneity, Their advantage over entropy change, Variation of *G* and *A* with *P, V* and *T*, Temperature dependence of free energy: Gibbs-Duhem, Gibbs-Margulesequation, Clausius-Clapeyron equation and its applications.

UNIT – IV **12 hours**

Chemical kinetics-I: Introduction to chemical kinetics, Order and molecularity of chemical reaction, Rate expression for first order, second order and third order reactions, Half life, Methods for determining order of reaction, Effect of temperature and catalyst on rate of reaction, Arrhenius equation, Concept of activation energy, Simple collision theory based on hard sphere model, Expression of rate constant based on equilibrium constant and thermodynamic aspects, Numericals.

Liquid states of matter: Structure and physical properties of liquid: vapor pressure, surface tension and viscosity, Numericals.

UNIT – V **12 hours**

Electrochemistry-I: Conductance and ionization: Review of electrolytes, Arrhenius theory of electrolytic dissociation, Conductance and its variation with dilution, Ionic mobility, Kohlrausch law and its applications.

Migration of Ions: Transport number and its relation with concentration and ionic mobility, Experimental procedures for measuring transport numbers (Hittorf's rule, Moving boundary method), Abnormal transport numbers, Walden's rule.

Applications of conductance measurements: Determination of degree of dissociation of weak electrolytes, ionic product of water, solubility and solubility product of sparingly soluble salts, Conductometric titrations.

REFERENCES

1. F. Daniels, *Mathematical preparation for physical Chemistry*, McGraw Hill Inc. US, 1959.
2. R.G. Mortimer, *Mathematics for Physical Chemistry*, Elsevier, 3rd Ed., 2011.
3. D. A. McCurrie, *Mathematics for Physical Chemistry: Opening Doors*, University Science Books, 2008.
4. E. Steiner, *The Chemistry Math Book*, Oxford, 2nd Ed., 2008
5. P. W. Atkins, *The Elements of Physical Chemistry*, Oxford, 10th Ed., 2016.
6. R. P. Rastogi and R. R. Mishra, *Chemical Thermodynamics*, Vikas Publishing House Pvt. Ltd., 6th Ed., 2009.
7. K. L. Kapoor, *A Text Book of Physical Chemistry*, McGraw Hill Education (India) Pvt. Ltd., Vol. 3, 5th Ed., 2014.
8. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Co., 47th Ed., 2017.

Semester: III
Course Name: Inorganic Chemistry Lab-I
Course Code: **3 Credits (0-0-6)**

PART A: Volumetric analysis
Complexometric titrations:
1. Estimation of Zn ions using EDTA.
2. Determination of Hardness of Water (Ca/Mg ions) using EDTA.

Iodometry and iodimetry redox titration:
1. Determination of strength of copper sulphate solution iodometrically using iodine solution.
2. Determination of strength of arsenous oxide solution iodimetrically using sodium thiosulphate solution.

PART B: Synthesis and analysis
1. Preparation of sodium trioxalato ferrate (III), $Na_3[Fe(C_2O_4)_3]$.
2. Preparation of Nickel dimethyl glyoxime Ni-DMG complex, $[Ni(DMG)_2]$.
3. Preparation of copper tetraammine complex, $[(Cu(NH_3)_4]SO_4$.
4. Preparation of *cis*-and *trans*-bisoxalato diaqua chromate (III) ion.

PART C: Gravimetric analysis
1. Estimation of calcium as calcium oxalate.
2. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.
3. Estimation of Copper as CuSCN.
4. Estimation of Ni(II) using dimethylgloxime.

REFERENCES

1. A. O. Thomas, *Practical Chemistry*, Scientific Book Centre, Cannanore, 2003.
2. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, *Basic Principles of Practical Chemistry*, 2nd Ed., Sultan Chand & Sons, New Delhi.
3. J. Mendham, R. C. Denny, J. D. Barnes and M. J. K. Thomas, *Vogel's Text Book of Quantitative Chemical Analysis*, 6th Ed., Prentice Hall.
4. G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denny, *Vogel's Textbook of Quantitative Analysis*, 5th Ed., John Wiley and Sons, 1989.
5. W. L. Jolly, *Synthesis and Characterization of Inorganic Compounds*, Prentice Hall, 1971.
6. In-house laboratory manual with experimental procedures and relevant information.

Semester: III
Course Name: Organic Chemistry Lab-I
Course Code: 3 Credits (0-0-6)

PART A: Organic preparations (At least 8 experiments)

1. Acetylation of one of the following compounds: Aniline, *o*-, *m*-, *p*-Toluidines, *o*-, *m*-, *p*-Anisidines, Phenols, β-Naphthol, Salicylic acid by (i) using conventional method and (ii) using green approach
2. Benzolyation of one of the following compounds: Aniline, *o*-, *m*-, *p*-Toluidines, *o*-, *m*-, *p*-Anisidines, Phenols, β-Naphthol, Resorcinol by Schotten-Baumann reaction
3. Oxidation of ethanol/ isopropanol (Iodoform reaction).
4. Bromination of acetanilide by conventional method and using green approach (Bromate-bromide method)
5. Bromination of aniline or phenol
6. Nitration of any one of the following: Acetanilide/nitrobenzene by conventional method.
7. Nitration of salicylic acid by green approach (using ceric ammonium nitrate).
8. Selective reduction of *m*- dinitrobenzene to *m*-nitroaniline.
9. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
10. Hydrolysis of amides and esters.
11. Semicarbazone of any one of the following compounds: Acetone, Ethyl methyl ketone, Cyclohexanone, Benzaldehyde.
12. Aldol condensation using either conventional or green method.

PART B: Separation of organic mixture (at least 4-6 mixtures)

The given mixture of organic compounds will be separated *via* biphasic extraction method. A binary mixture containing strongly acidic, weakly acidic, basic and neutral compounds will be provided from the following list.

1. Strongly acidic compounds: Carboxylic acids, Sulphonic acids
2. Weakly acidic compounds: Phenols, Naphthols
3. Basic compounds: Amines
4. Neutral compounds: Hydrocarbons, Carbohydrates, Amides, Diamides, Esters, Nitrocompounds, Halogen compounds, etc.

REFERENCES

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry,* 5th Ed., Pearson, 2012.
2. In-house laboratory manual with experimental procedures and relevant information.

Semester: IV
Course Name: Inorganic Chemistry-II
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**
Chemistry of transition elements-I: General characteristic properties of 3*d*-block elements, Relative stability of their oxidation states with special reference to electronic configuration, Atomic radii and ionic radii, Oxidation state, Colour, Ionization enthalpy, Ability to form complexes, Magnetic properties, Catalytic properties, Formation of binary compounds-Oxides, Halides and sulphides, Coordination number, Geometry and complex formation.

UNIT – II **12 hours**
Chemistry of transition elements-II: General characteristic properties of 4*d*- and 5*d*-block elements, Comparative treatment with 3*d*-analogues with special reference to electronic configuration, Atomic radii and ionic radii, Colour, Variable valency, Ability to form complexes, Magnetic and catalytic properties, Difference between 3*d*-, 4*d*- and 5*d*-transition series. Position of lanthanides and actinides in the periodic table, Lanthanide contraction, Spectral and magnetic properties of lanthanides, Separation of lanthanides and actinides.

UNIT – III **12 hours**
Acids and bases: Acid-base theories: Arrhenius, Bronsted-Lowry, Lewis, Lux-Flood, Usanovich, Hard and soft acids and bases (HSAB), Classification of acids and bases as hard and soft, Pearson's HSAB concept, Acid-base strength in relation to hardness and softness, Symbiosis, Theoretical basis of hardness and softness, Relationship between electronegativity and hardness/softness.

UNIT – IV **12 hours**
Chemistry of non-aqueous solvents: Physical properties of a solvent, Solvent system and its classification, Reactions in non-aqueous solvents with reference to liquid NH_3, H_2SO_4, liquid HF, liquid SO_2. PCl_5, Chemistry of molten salts as non-aqueous solvents: Solvent properties, solution of metals, complex formation, Low temperature molten salts, Super acids, Supercritical fluids: Properties of supercritical fluids and their uses as solvents.

UNIT – V **12 hours**
Nuclear chemistry and radioactivity-I: Fundamental particles of nucleus, Basics of different nuclear models (shell model, liquid drop model, fermi gas model, collective model), Isotone, Isobar and Nuclear isomer, Nuclear reactions, Types of nuclear reactions, Chemical effects of nuclear transformations, Nuclear fission and nuclear fusion, Fission products and fission yields, IsotopeNuclear reactors: Classification of reactors, Reactor power, Nuclear waste management.

REFERENCES

1. F. A. Cotton and G. Wilkinson, *Basic Inorganic Chemistry*, 6th Ed., John Wiley.
2. J. E. Huhey, Harpes and Row, *Inorganic Chemistry*, 4th Ed., 2006.
3. G. Wilkinson, R. D. Gillars and J. A. Mccleverty, *Comprehensive Coordination Chemistry,* Pergamon, 1987.
4. J. D. Lee, *Concise Inorganic Chemistry*, 5th Ed., 2006.
5. N. N. Greenwood and Earnshop, *Chemistry of the Elements*, 2nd Ed., Pergamon, 1997.
6. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed., 1993.

7. B. R. Puri, L. R. Sharma and K. K. Kalia, *Principles of Inorganic Chemistry*, 23rd Ed., New Delhi, Shoban Lal Nagin Chand & Co, 1993.
8. D. F. Shriver and P. W. Atkins, *Inorganic Chemsitry*, 1999.
9. H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Ed., Wiley Eastern, 1987.
10. G. Friedlander, T. W. Kennedy, E. S. Macias and J. M. Miller, *Introduction of Nuclear and Radiochemistry*, 3rd Ed., John Wiley, 1981.

Semester: IV
Course Name: Organic Chemistry-II
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Alcohols: Monohydric alcohols: Methods of formation, Reduction of aldehydes, ketones, carboxylic acids and esters, Hydrogen bonding, Acidic nature, Reactions of monohydric alcohols: Substitution, Dehydration, Oxidation and Esterification, Methods to distinguish primary, secondary and tertiary alcohols, Dihydric alcohols: Methods of formation, Chemical reactions of vicinal glycols, Oxidative cleavage by periodic acid and lead tetraacetate, Pinacol-pinacolone rearrangement, Trihydric alcohols: Methods of formation, chemical reactions of glycerol.

UNIT – II 12 hours

Phenols: Preparation of phenols, Acidity and factors effecting it, Relative acidity of phenol, alcohol and carboxylic acid, Resonance stabilization of phenoxide ion, Reactions of phenols, Electrophilic aromatic substitution, Mechanisms of Fries rearrangement, Claisen rearrangement, Kolbe's–Schmidt reaction, Gattermann synthesis, Hauben-Hoesch, Lederer-Manasse and Reimer-Tiemann reaction Schotten-Baumann Reaction.

UNIT – III 12 hours

Ethers: Nomenclature, Methods of formation, Physical properties, Chemical reactions, Cyclic ethers, Introduction to crown ethers, Structure and applications.
Epoxides: Nomenclature and synthesis of epoxides, Acid and base-catalyzed ring opening of epoxides, Regiochemistry of epoxide ring opening, Reactions of epoxides with alcohols, amines, Grignard and organolithium reagents.

UNIT – IV 12 hours

Alkyl halides: Methods of formation, Mechanisms of nucleophilic substitution reactions of alkyl halides (S_N1, S_N2, S_Ni), Substitution at the allylic and vinylic positions, Mechanisms of elimination reactions of alkyl halides (E1 and E2), Stereochemical aspects of substitution and elimination reactions, Competition between substitution and elimination, Relative reactivities of alkyl halides vs allyl, vinyl and aryl halides.
Aryl halides: Preparation of aryl halides, Aromatic nucleophilic substitution, Addition-elimination and the elimination-addition mechanisms.

UNIT – V 12 hours

Carboxylic acids: Nomenclature, structure and bonding, Preparation of monocarboxylic acids, Physical properties, Acidity of carboxylic acids, Effect of substituents on acid strength, Reactions of carboxylic acids, HVZ reaction, Synthesis of acid chlorides, esters and amides, Reduction of carboxylic acids, Mechanism of decarboxylation, Methods of formation and chemical reactions hydroxy acids: Malic, Tartaric and Citric acids, Dicarboxylic acids, Methods of formation and effect of heat and dehydrating agents, Unsaturated acids: Cinnamic, Maleic and Fumaric acids.
Carboxylic acid derivatives: Preparation and reactions of acid chlorides, anhydrides, esters, amides and acid anhydrides, Comparative study of nucleophilic substitution at acyl group, Mechanism of acidic and alkaline hydrolysis of esters, Claisen and Dieckmann condensations, Reformatsky reaction, Hofmann bromamide degradation, Curtius rearrangement.

REFERENCES

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Ed., 2010.
2. T. W. Graham Solomons, *Fundamentals of Organic Chemistry*, John Wilev, 5th Ed., 1998.
3. Streitwiesser, Hathcock and Kosover, *Introduction to Organic Chemistry*, Macmillan, 4th Ed., 1992.
4. I. L. Finar, *Organic Chemistry*, Vol. I and II, 6th Ed., 2002.
5. P. Sykes, *A Guide Book to Mechanism in Organic Chemistry*, 6th Ed., 2003.
6. S. H. Pine, *Organic Chemistry*, 5th Ed., 2007.
7. M. B. Smith, *March's Advanced Organic Chemistry, Reactions, Mechanisms and Structure*, 7th Ed., 2016.
8. P. S. Kalsi, *Organic Reactions and their Mechanisms*, 4th Ed., New Age International, 2017.

Semester: IV
Course Name: Physical Chemistry II
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Chemical equilibrium: Dynamic nature of Chemical equilibrium, Attainment and characteristics of chemical equilibrium, Law of mass action and its thermodynamic derivation, Relation between K_p, K_c and K_x, Thermodynamic relations for chemical affinity, Homogeneous equilbria, Temperature dependence of equilibrium constant and integrated form of van't Hoff equation, Pressure dependence of equilibrium constant (K_p, K_c and K_x), Heterogeneous equilibria, Le Chatelier's principle, Thermodynamic treatment of Le Chatelier's principle.

UNIT – II **12 hours**

Phase equilibrium: Statement and meaning of the terms – phase, component and degree of freedom, Conditions for equilibrium between phases, Thermodynamic derivation of Gibbs Phase Rule, Phase equilibria of one component system: water, carbon dioxide and sulphur systems, Phase equilibria of two component systems: simple eutectic systems like Pb-Ag system, Compound formation with congruent m.pt. Mg-Zn and $FeCl_3$-H_2O system, Compound formation with incongruent m.pt., Liquid-liquid mixtures: ideal liquid mixtures, Raoult's and Henry's Law, Non ideal systems, Azeotropes, HCl-Water and ethanol-water systems, Partially miscible liquids: phenol-water system.

Nernst distribution law: Partition coefficient, Thermodynamic derivation, Association and dissociation of solute in one solvent.

UNIT – III **12 hours**

Electrochemistry II: E.M.F. and potential, Nernst equation, Derivation of cell E.M.F. and single electrode potential.

Reference electrode: Standard hydrogen electrode, Ag/AgCl and Calomel electrode, Electrolytic and Galvanic cells: Reversible and irreversible cells, Calculation of thermodynamic quantities of cell reactions (ΔG, ΔH and K).

Formal potential and its application: Effect of pH, Concentration cell with and without transport, Liquid junction potential, Application of EMF measurement: Solubility product and activity coefficient, Potentiometric titrations (redox and acid-base), Determination of pH using hydrogen and quinhydrone electrodes by potentiometric methods.

UNIT – IV **12 hours**

Catalysis: Characteristic of catalytic reactions, Homogeneous catalysis, Acid-base catalysis and its kinetics, Enzyme catalysis and its mechanism, Effect of temperature on enzyme catalysis, Heterogeneous catalysis, Surface reactions, Kinetics of surface reactions, Unimolecular surface reactions, Bimolecular surface reactions, Effect of temperature on heterogeneous reactions: Unimolecular and bimolecular.

UNIT – V **12 hours**

Solid state chemistry: Crystal structures, Close packing, Body centered and primitive structures, Symmetry in crystals, Crystallographic point groups, Space groups, Lattices, One, Two- and Three-dimensional unit cells, Translational symmetry elements, Miller & Weiss indices, Interplanar spacing, Packing diagrams, Atomic packing fraction, Braggs' law, Structures of important ionic solids: Ionic Radii, Ionic solids with formula MX (CsCl, NaCl, zinc blende and wurtzite structures), MX_2 (fluorite and anti-fluorite structures), Crystal defects.

REFERENCES

1. P. W. Atkins, *The Elements of Physical Chemistry*, Oxford, 10th Ed., 2016.
2. R. P. Rastogi and R. R. Mishra, *Chemical Thermodynamics*, Vikas Publishing House Pvt. Ltd., 6th Ed., 2009.
3. K. L. Kapoor, *A Text Book of Physical Chemistry*, McGraw Hill Education (India) Pvt. Ltd., Vol. 3, 5th Ed., 2014.
4. S. Glasstone, *An Introduction to Electrochemistry*, Affiliated East-West Press Pvt. Ltd., New Delhi, 2006.
5. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Co., 47th Ed., 2017.
6. A. R. West, *Solid State Chemistry*, Wiley Student Ed., (Indian Ed.), 2003.
7. I. N. Levin, *Physical Chemistry*, Mc Graw Hill Education, 6th Ed., 2011.
8. C. N. R. Rao and J. Gopalakrishnan, *New Directions in Solid State Chemistry*, Cambridge University Press, 2nd Ed., 1987.

Semester: IV
Course Name: Organic Chemistry Lab-II
Course Code: **4 Credits (0-0-8)**

PART A: Quantitative estimation of organic compounds:

1. Estimation of aniline (Bromate-bromide method)
2. Estimation of glucose (Fehling's method)
3. Estimation of phenol (Bromate-bromide method)
4. Estimation of ascorbic acid in Vitamin C tablets
5. Estimation of amino acid

Part B: Qualitative analysis of organic compounds (At least six compounds)

Identification of organic compounds via systematic functional group analysis: Phenols, Carboxylic acids, Aldehydes, Ketones, Carbohydrates, Aromatic amines, Esters, Amides etc.

REFERENCES

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry,* 5th Ed., Pearson, 2012.
2. In-house laboratory manual with experimental procedures and relevant information.

Semester: IV
Course Name: Physical Chemistry Lab-I
Course Code: **4 Credits (0-0-8)**

PART A: Electrochemistry

1. Determination of the molar conductivity of weak monobasic acid over a given range of concentration.
2. Determination of the Ionization constant of a weak acid conductometrically.
3. Study the conductometric titration of strong acid Vs strong base.
4. Potentiometric titration of an acid with a base.
5. Determination of the pK_a value of the given organic acid by pH measurement.

PART B: Liquid state

1. Determination of the surface tension of a liquid by stalagmometer method
2. Determination of the viscosity of a given liquid by Oswald's viscometer

PART C: Thermochemistry

1. Determination of the heat of neutralization of HCl by NaOH

PART D: Kinetics

1. Study the kinetics of hydrolysis of an ester in presence of HCl as catalyst
2. Determination of equilibrium constant of the reaction $KI + I_2 \rightleftharpoons KI_3$ by solubility method

PART E: Phase equilibrium

1. Determination of the distribution coefficient (partition coefficient) of benzoic acid between benzene and water at room temperature.
2. Determination of the distribution coefficient (partition coefficient) of iodine between two immiscible solvents (H_2O-C_6H_6; H_2O-CCl_4).

REFERENCES

1. A. Ghoshal, B. Mahapatra and A. K. Nad, *An Advanced Course in Practical Chemistry,* New Central Book Agency Pvt. Ltd., 3rd Ed., 2012.
2. B. P. Levitt, *Findley's Practical Physical Chemistry*, Longman Group Limited, 9th Ed., 1954.
3. J. B. Yadav, *Advanced Practical Physical chemistry*, Goel Publishing, 1st Ed., 2015.
4. B. Viswanathan and P. S. Raghavan, *Practical Physical chemistry*, Viva Books Pvt. Ltd., 1st Ed., 2014.
5. In-house laboratory manual with experimental procedures and relevant information.

Semester: IV
Course Name: Basic Analytical Chemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Analytical methods: Types of analytical methods, Importance of analytical methods in qualitative and quantitative analysis, Chemical and instrumental methods, Advantages and limitations of chemical and instrumental methods.
Laboratory hygiene and safety: Storage and handling of corrosive, flammable, explosive, toxic, carcinogenic and poisonous chemicals, Simple first aid procedures for accidents involving acids, alkalies, bromine, burns and cut by glass, Threshold vapour concentration, Safe limits, Waste disposal and fee me disposal.

UNIT – II 12 hours
Errors in chemical analysis: Accuracy and precision of measurements, Determinate indeterminate, Systematic and random errors in chemical analysis with examples, Absolute and relative errors, Source, Effect and Detection of systematic errors, Distribution of random errors, Normal error curve, Standard deviations, Standard deviation of calculated results: Sum or difference, Product or quotient, Significant figures, Rounding and expressing results of chemical computations.

UNIT – III 12 hours
Solvent extraction: Solvent purification methods, Distribution law, Single extraction, Multiple extraction, Craig concept of counter-current distribution, Important solvent systems: Chelate extraction, Synergic extraction, Extraction by solvation, Ion-pair extraction
Radio-analytical methods: Elementary theory, Isotope dilution and Neutron activation methods and applications.

UNIT – IV 12 hours
Chromatographic techniques: Chromatographic separations: General description and classification of chromatographic methods, Thin layer, Paper and Column chromatographic techniques and their simple applications, Types of adsorbents, R_f-values and their significance, Elution in column chromatography, Migration rates of solutes, Band broadening and column efficiency, Column resolution, Ion exchange resins and their exchange capacities, Principle and simple applications of ion exchange separation.

UNIT – V 12 hours
Thermo analytical methods: Principles and applications of Thermogravimetry Analysis (TGA), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Thermometric titrations.

REFERENCES

1. J. Mendham, R. C. Denney, J. D. Barnes and M. J. K. Thomas, *Vogel's Quantitative Chemical Analysis*, 6th Ed., Pearson, 2009.
2. H. H. Willard, L. L. Merritt Jr., J. A. Dean and F. A. Settle Jr., *Instrumental Methods of Analysis*, 7th Ed., Wardsworth Publishing Company, 1988.
3. G. D. Christian, *Analytical Chemistry*, 6th Ed., John Wiley & Sons, New York, 2004.
4. D. C. Harris, *Exploring Chemical Analysis*, 9th Ed., New York, W.H. Freeman, 2016.
5. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, 3rd Ed., New Age International Publisher, 2008.

6. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, 7th Ed., 2006.
7. O. Mikes, *Mikes Laboratory Hand Book of Chromatographic and Allied Methods (Elles Harwood Series on Analytical Chemistry)*, John Wiley & Sons, 1979.

Semester: V
Course Name: Organic Spectroscopy and Compounds with Heteroatoms
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**
UV-Vis spectroscopy: Introduction, Absorption laws, Instrumentation, Formation of absorption bands, Types of electronic transitions, Chromophores, Auxochromes, Absorption and intensity shifts, Solvent effects, Woodward-Fieser rules for calculating absorption maximum in dienes and α,β-unsaturated carbonyl compounds.
IR spectroscopy: Introduction, Theory of molecular vibrations, Vibrational frequency, Factors influencing vibrational frequencies, Finger print region, Applications of IR spectroscopy in functional group analysis, Effect of hydrogen bonding, conjugation, resonance and ring size on IR absorptions.

UNIT – II **12 hours**
NMR Spectroscopy: Basic principles of proton magnetic resonance, Instrumentation, Number of signals, Position of signals (Chemical shift), Shielding and deshielding effects, Factors influencing chemical shifts: Inductive effect, Anisotropic effect in alkenes, alkynes, aldehydes and aryl compounds, Hydrogen bonding, Splitting of signals, Spin-spin coupling, Coupling constant, Introduction to ^{13}C NMR.

UNIT – III **12 hours**
Introduction to mass spectrometry: Instrumentation, Ionization, Fragmentation, Molecular ion peak, Base peak, Isotopic peaks, Nitrogen rule, McLafferty rearrangement, Retro Diels-Alder reaction.
Applications of spectral techniques: Structural determination of simple organic compounds using UV, IR and NMR spectral data.

UNIT – IV **12 hours**
Nitro compounds: Preparation of nitroalkanes and nitroarenes, Chemical reactions of nitroalkanes, Mechanism of nucleophilic substitution in nitroarenes, Picric acid.
Amines: Preparation of alkyl and aryl amines *via* reduction of nitro compounds and nitriles, Reductive amination, Hofmann degradation, Gabriel-phthalimide reaction, Hoffmann rearrangement, Separation of a mixture of primary, secondary and tertiary amines (Hinsberg's method), Reactions of amines, Electrophilic aromatic substitution, Basicity of amines and effect of substituents on basicity, Amine salts as phase transfer catalysts, **Diazonium salts**: Preparation and reactions.

UNIT – V **12 hours**
Organosulfur compounds: Nomenclature, Methods of formation of thiols, thioethers, sulphonic acids, sulphonamides, suphur ylides, thiocyanates, isothiocyanates and sulphaguanidine.
Organophosphorus and organosilicon compounds: Preparation and chemical reactions of organophosphorous and organosilicon compounds, Phosphines, Phosphorous ylides, Wittig reaction, Phophine oxides, Esters of phosphorous acids, Alkyl silanes, Silanols, Siloxanes, Silylamines, Hiyama coupling.

REFERENCES

1. W. Kemp, *Organic Spectroscopy*, 3rd Ed., 1991.

2. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., 2017.
3. R. M. Silverstein, F. X. Webster and D. V. Kiemle, *Spectrometric Identification of Organic Compounds*, 8th Ed., 2014.
4. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 6th Ed., 2007.
5. J. Mohan, *Organic Spectroscopy, Principles and applications*, 2nd Ed., 2001.
6. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Ed., 2010.
7. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry: Part A: Structure and Mechanisms*, 5th Ed., 2008.
8. I. L. Finar, *Organic Chemistry*, Vol. I and II, 6th Ed., 2002.
9. S. H. Pine, *Organic Chemistry*, 5th Ed., 2007.

Semester: V
Course Name: Quantum Mechanics, Surface and Colloidal Chemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Basics of quantum mechanics-I: Basic principles of quantum mechanics, Inadequacy of classical mechanics, The concept of quantization, Black–body radiation, Planck's radiation law, Photoelectric effect, Heat capacity of solids, Bohr's model of hydrogen atom and its defects, Compton effect, The wave-particle duality, The Heisenberg's uncertainty principle, Operator formalism: Linear operator, Hermitian operator and angular momemtum operator, Commutator, Eigen functions and eigen values, Expectation values.

UNIT – II 12 hours
Basics of quantum mechanics-II: Hamiltonian operator, Schrödinger wave equation and its importance, Physical interpretation of the wave function, Orthogonal and orthonormal functions, Correspondence principle, Postulates of quantum mechanics and their analysis, Particle in a one, two and three-dimensional box, Degeneracy and its applications to conjugated systems.

UNIT – III 12 hours
Application of quantum mechanics: Simple harmonic oscillator: Setting up of the Schrodinger stationary equation, Energy expression (without derivation), Expression of wave function for $n = 0$ and $n = 1$ (without derivation) and their characteristic features; Schrödinger wave equation for *H*-atom, Transformation of coordinates: Cartesian to polar (without derivation), Separation into three total differential equations in terms of the variables r, θ, φ; and their significance, Solution of φ equation and emergence of magnetic quantum number 'm', Concept of orbital.

UNIT – IV 12 hours
Surface chemistry: Structure of solid surfaces: Adsorption and desorption of molecules, physisorption and chemisorption, Surface reaction kinetics, Langmuir, BET and Freundlich adsorption isotherms, The rates of surface processes, Temperature dependence of adsorption, Structure of heterogeneous surfaces: Langmuir-Hinshelwood and Eley-Rideal mechanism.

UNIT – V 12 hours
Colloidal state: The colloidal systems, general properties, Tyndall effect, Properties of hydrophobic colloidal systems: Electrical properties (electrical double layer) and electrokinetic properties (electro-osmosis).
Surface active agent, Classification of surface active agent, Critical micelle concentration (CMC), Factor affecting the CMC of surfactants, Hydrophobic interaction, Thermodynamics approach to CMC and micellization.

REFERENCES

1. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach*, Viva Student Ed., 2011.
2. D. A. McQuarrie, *Quantum Chemistry,* Viva Student Ed., 2014.
3. R. K. Prasad, *Quantum Chemistry*, New Age International Publishers Ltd., New Delhi, 4th revised Ed., 2014.
4. A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw Hill, 4th Ed., 1998.
5. I. N. Levine, *Quantum Chemistry*, Pearson, 7th Ed., 2013.

6. P. W. Atkins and J. de Paula, *The Elements of Physical Chemistry*, Oxford, 10th Ed., 2014.
7. P. W. Atkins and R. Friedman, *Molecular Quantum Mechanics*, Oxford University Press, 5th Ed., 2012.
8. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Co., 47th Ed., 2017.
9. Y. Moroi, *Micelles: Theoretical and Applied Aspects,* Springer, 1992 Ed.

Semester: V
Course Name: Seminar
Course Code: **2 Credits (0-0-4)**

As part of this interactive course mentored by a faculty, the learners will be required to present the key research questions addressed, experimental design and major results from any recent publication in a reputed peer reviewed journal on any aspect of Chemistry – Organic, inorganic, physical, analytical or inter-disciplinary chemistry. The students will deliver a power point presentation at the end of semester examination.

Semester: V
Course Name: Physical Chemistry Lab-II
Course Code: **3 Credits (0-0-6)**

Part A: Conductometry

1. Determination of the saponification of ethyl acetate conductometrically.
2. Determination of the strength of the given acid condutometrically using standard alkali solution.
    a. Weak acid - Strong base
    b. Weak acid - Weak base
    c. Strong acid - Weak base
3. Potentiometric titration of KCl, KBr and their mixture with $AgNO_3$ solution.
4. Determination of pH of buffer solutions potentiometrically.

Part B: Spectroscopy

1. Determination of the specific rotation of a given optically active compound.
2. Verify Beer- Lambert Law for a coloured solution ($KMnO_4/K_2Cr_2O_7$).
3. Determination of indicators constant (pK_{In}) of methyl red colorimetrically.
4. Determination of the λ_{max} for $KMnO_4$ by colorimetric measurements.

Part C: Adsorption

1. Determination of adsorption of acetic acid on charcoal - verification of Freundlich's adsorption isotherm.
2. Determination of the adsorption of oxalic acid by activated charcoal and test the validity of Freundlich/Langmuir Isotherms.

Part D: Kinetics

1. Determination of the kinetics of decomposition of H_2O_2.

Part D: Computer in chemistry

1. Study of simple control commands of *vi* editor embedded in a Linux box.
2. Plotting a linear graph using MS excel and Xmgrace from a given set of data set.
3. Plotting a non-linear graph using a given data set.
4. Study of quantum chemistry using computational chemistry software:
    a. Determination of the Z-matrices (Cartesian coordinate) of simple molecules: H_2, H_2O, H_2O_2, HCHO, etc.
    b. Drawing 3D structures of complex molecules using GaussView and determination of Z-matrices.
    c. Optimization and frequency calculation using Gaussian 16 software using GaussView as a tool.

REFERENCES

1. A. Ghoshal, B. Mahapatra and A. K. Nad, *An Advanced Course in Practical Chemistry,* New Central Book Agency Pvt. Ltd., 3rd Ed., 2012
2. J. B. Yadav, *Advanced Practical Physical chemistry*, Goel Publishing, 1st Ed., 2015.
3. B. Viswanathan and P. S. Raghavan, *Practical Physical chemistry*, Viva Books Pvt. Ltd., 1st Ed., 2014.
4. In-house laboratory manual with experimental procedures and relevant information.

Semester: V
Course Name: Properties of Inorganic Metal Complexes
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Electronic spectra of transition metal complexes-I: Quantum numbers, Types of electronic transitions, Selection rules for *d-d* transitions, Spectroscopic ground states, Term symbols, Microstates, Spectrochemical series of ligands, Orbital and spin magnetic moments, Orbital contribution, Quenching of magnetic moment, Russel-Saunders Coupling: *l-l* coupling, *J-J* coupling, *L-S* coupling, Derivation of Russell-Saunders terms: p^2, d^2 configuration, Orgel-energy level diagram for d^1 to d^9 states, Discussion of the electronic spectrum of $[Ti(H_2O)_6]^{3+}$ complex ion, Nepheleuxatic effect.

UNIT – II 12 hours

Magnetic properties of transition metal complexes-I: Definition of magnetic properties, Types of magnetic bodies (Diamagnetism, Paramagnetism Ferromagnetism and Anti-ferromagnetism, Mechanism of anti-ferromagnetic interaction, Spin-only formula, Spin orbit coupling, Lande interval rule, Energies of *J* levels, Curie equation, Curie and Curie-Weiss law, Temperature independent paramagnetism, Derivation and application of Van Vleck susceptibility equation, Magnetic exchange coupling and spin crossover (Low spin and high spin cross over), Correlation of magnetic moment data and stereochemistry, Anomalous magnetic moments, Magnetic properties of binuclear and polynuclear complexes.

UNIT – III 12 hours

Magnetic properties of transition metal complexes-II: Magnetic susceptibility-orbital and spin effects, Importance of magnetic susceptibility, Diamagnetism and Pascals's constant, Gouy's method, Faraday method, Vibrating sample magnetometer, SQUID, NMR method for measuring magnetic susceptibility, Correlation of μs and μeff values, Orbital contribution to magnetic moments, Magnetic properties based on crystal field models: Octahedral, Tetrahedral, Trigonal bipyramidal, Square pyramidal and tetragonally distorted octahedral complexes, Diamagnetism in atoms and polynuclear systems.

UNIT – IV 12 hours

Metal π-complexes–I: Metal carbonyls, Classification of metal carbonyls, Effective atomic number, Preparation and important reactions (substitution, nucleophilic, electrophilic, reduction reactions) of metal carbonyls, Structure and chemical bonding in metal carbonyls, Preparation of anionic metal carbonyl complexes and Substituted metal carbonyl complexes, Vibrational spectra of metal carbonyls for bonding and structural elucidation, Application of metal carbonyls complexes.

UNIT – V 12 hours

Metal π-complexes–II: Dinitrogen as ligands and dioxygen complexes-Preparation, Structure, Bonding, and important reactions with transition metals, Metal nitrosyls complexes-Preparation, Structure, Bonding, and important reactions with transition metals, Ligating behaviour of tertiary phosphines, Isopoly and heteropoly acids-salts of molybdenum and tungsten.

REFERENCES

1. F. A. Cotton and G. Wilkinson, *Basic Inorganic Chemistry*, 6th Ed., John Wiley, 2003.

2. J. E. Huhey, Harpes and Row, *Inorganic Chemistry*, 4th Ed., Pubs: Harper Collins 2006.
3. G. Wilkinson, R. D. Gillars and J. A. Mccleverty, *Comprehensive Co-ordination Chemistry,* Pergamon, 1987.
4. J. D. Lee, *Concise Inorganic Chemistry*, 5th Ed., John Wiley & Sons, 1996.
5. D. F. Shriver, F. W. Atkins and C. M. Langford, *Inorganic Chemistry*, 3rd Ed., Oxford University Press, 1999.
6. A. G. Massey, *Main Group Chemistry*, Ellis Horwood, New York, 1990.
7. B. R. Puri, L. R. Sharma and K. C. Kalia, *Text Book of Inorganic Chemistry*, Sultan Chand & Sons, New Delhi 1993.
8. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, Elsevier Applied Science, 1968.
9. Malik, Tuli and Madan, *Selected Topics in Inorganic Chemistry*, S. Chand & company, New Delhi, 2002.
10. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, Oxford University Press, 2006.
11. A. Earnshaw, *Introduction to Magnetochemistry*, 1st Ed., Academic Press, 1968.
12. R. L. Carlin, *Magnetochemistry*, SpringerVerlag, Berlin, 1986.
13. A. Syamal and R. L. Dutta, *Elements of Magnetochemistry*, East-West Press Pvt. Ltd.
14. F. E. Mabbs, D. J. Machin, *Magnetism and Transition Metal Complexes*, Springer, 1973.

Semester: V
Course Name: Natural Products Chemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**
Carbohydrates: Classification, Chemistry of monosaccharides (glucose and fructose), Mechanism of osazone formation, Interconversion of glucose and fructose, Chain lengthening and chain shortening of aldoses, Configuration of monosaccharides, Erythro and threo diastereomers, Mechanism of mutarotation, Introduction to disaccharides (maltose, sucrose and lactose) and polysaccharides (starch and cellulose) without involving structure determination, Industrial applications of starch and cellulose.

UNIT – II **12 hours**
Terpenoids: Classification, Isoprene rule, General methods of structural elucidation, Synthesis and stereochemistry of Citral, Geraniol and Menthol.
Carotenoids: Introduction, Structural elucidation and total synthesis of β-carotene.

UNIT – III **12 hours**
Alkaloids: Natural occurrence, General structural features, Physiological action, Occurrence and isolation, General methods of structural determination, Hoffmann's exhaustive methylation, Emde's modification, Synthesis of Coniine, Nicotine and Piperine.

UNIT – IV **12 hours**
Steroids: Occurrence, Nomenclature, Basic skeleton, Diel's hydrocarbon, Stereochemistry, Isolation, Structural determination and synthesis of Cholesterol and Estrone.

UNIT – V **12 hours**
Plant pigments: Occurrence, General methods of structural determination of Flavones and Isoflavones, Synthesis of Quercetin, Cyanidin and Cyanin, Biosynthesis of flavonoids: Acetate pathway.

REFERENCES
1. J. Mann, R. S. Davidson, J. B. Hobbs, D.V. Banthrope and J. B. Harborne, *Natural Products: Their Chemistry and Biological Significance*, Harlow, Essex, England Longman Scientific & Technical, New York, Wiley, 1st Ed., 1994.
2. M. Nogradi, *Stereoselective Synthesis A Practical Approach*, 2nd Ed., 1994, VCH.
3. K. Hostettmann, M. P. Gupta and A. Marston, *Chemistry, Biological and Pharmacological Properties of Medicinal Plants From the Americas*, 1997, Harwood Academic Publishers.
4. B. A. Bohm, *Introduction to Flavonoids*, 1998, Harwood Academic Publishers.
5. Atta-ur-Rahman M. I. Choudhary, *New Trends in Natural Product Chemistry*, 1998, Harwood Academic Publishers.
6. S. Dev, *Insecticides of Natural Origin*, 1997, Harwood Academic Publishers.
7. I. L. Finar, *Organic Chemistry*, Vol. II, 3rd Ed., 1964.

Semester: V
Course Name: Inorganic Chemistry Lab-II
Course Code: **3 Credits (0-0-6)**

PART A: Qualitative inorganic analysis
Qualtative semimicro analysis of mixture containing three anion radicals and three cation radicals.
Analysis of anions: Acetate, Oxalate, fluoride, Chloride, Bromide, Iodide, Nitrate, Carbonate, Sulphide, Sulphite, Sulphate, Borate and Phosphate.
Analysis of cations: NH_4^+, Pb^{2+}, Bi^{3+}, Cu^{2+}, Cd^{2+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Ni^{2+}, Co^{2+}, Ca^{2+}, Ba^{2+}, Sr^{2+}, Mg^{2+}.
Mixture should preferably contain on interfering anion, or insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) or combination of anions CO_3^{2-} and SO_3^{2-}, NO^{2-} and NO^{3-}, Cl^- and Br^-, Cl^- and I^-, Br^- and I^-, NO^{3-} and Br^- and NO^{3-} and I^-.

PART B: Separation and quantitative estimation of two metal ions
1. Cu-Ni: Estimation of both by gravimetric method.
2. Cu-Zn: Estimation of both by gravimetric method.
3. Ni-Zn: Estimation of both by gravimetric method.
4. Cu-Fe: Estimation of both by gravimetric method.
5. Ba-Cu: Estimation of Ba gravimetrically and Cu volumetrically.
6. Ag-Cu: Estimation of Ag gravimetrically and Cu volumetrically.

REFERENCES
1. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, *Basic Principles of Practical Chemistry*, 2nd Ed., Sultan Chand & Sons, New Delhi.
2. J. Mendham, R. C. Denny, J. D. Barnes and M. J. K. Thomas, *Vogel's Text Book of Quantitative Chemical Analysis*, 6th Ed., Prentice Hall.
3. G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denny, *Vogel's Textbook of Quantitative Analysis*, 5th Ed., John Wiley and Sons, 1989.
4. G. R. Chatwal, *Instrumental Methods for Chemical Analysis*, 5th Ed., Himalaya Publications (India).
5. W. L. Jolly, *Synthesis and Characterization of Inorganic Compounds*, Prentice Hall.
6. In-house laboratory manual with experimental procedures and relevant information

Semester: VI
Course Name: Selected Topics in Inorganic Chemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**
Oxidation and reduction: Oxidation number, Redox potential, Half-cell reaction, Nernst equation (without derivation), Electrochemical series, Use of redox potential data–Analysis of redox cycle, Redox stability in water, Latimer diagram for oxygen, copper (acidic medium) and for chlorine (acidic/alkaline medium), Calculation of E values for skip-step couples using EMF diagrams, Frost diagrams for oxygen and nitrogen, Pourbiax diagram for iron couple, Applications of redox reactions to the extraction of elements from their ores: Ellingham diagrams.

UNIT – II **10 hours**
Chemistry of lanthanides elements: Position of lanthanides in the periodic table, Electronic structure, Oxidation states, Ionic radii and lanthanide contraction, Magnetic and spectral properties, Complex formation, Occurrence and isolation, Application of lanthanides.

UNIT – III **12 hours**
Chemistry of actinides elements: Position of actinides in the periodic table, Electronic structure, Oxidation states, Ionic radii, Magnetic and spectral properties, Complex formation, Occurrence and isolation, Separation of lanthanides: Ion-exchange method, General features and chemistry of actinides, Principles of separation of Np, Pu and Am from U, Application of actinides, Trans-uranium elements.

UNIT – IV **12 hours**
Nuclear chemistry and radioactivity-II: Introduction to radioactivity: Radioactive decay and equilibrium, Q value, Cross sections, Radioactive techniques, Tracer technique, Neutron activation analysis, Counting techniques such as G.M. ionization and proportional counter, Radioactive disintegration, Half life, Average life, Artificial transmutation, Decay kinetics, Types of decay, α-, β-, γ-emissions, Different radioactive series (natural and artificial), Group displacement law, Chemical reaction pathways and dating techniques, Mass defect and binding energy, Application of radioactivity and radio isotopes as tracers in analysis, in medicines, in biological field, in agriculture and in carbon dating.

UNIT – V **14 hours**
General principles of bioinorganic chemistry: A brief introduction to bioinorganic chemistry, Classification of elements (essential and trace) according to their action in biological system with special reference to Na^+, K^+ and Mg^{2+} ions, Generation of concentration gradients (Na^+/K^+ pump), Nitrogenase, Biological nitrogen fixation, Chemical nitrogen fixation, Role of Mg^{2+} ion in energy production and chlorophyll, Dioxygen transport and storage, Hemoglobin and Myoglobin-Electronic and spatial structures, Stabilization of protein structures and protein role(bones).

REFERENCES

1. A. Earnshaw, *Introduction to Magnetochemistry*, 1st Ed., Academic Press, 1968.
2. R. L. Carlin, *Magnetochemistry*, SpringerVerlag, Berlin, 1986.
3. A. Syamal and R. L. Dutta, *Elements of Magnetochemistry*, East-West Press Pvt. Ltd.
4. F. E. Mabbs, D. J. Machin, *Magnetism and Transition Metal Complexes*, Springer, 1973.

5. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, Oxford University Press, 2006.
6. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Ed., Pearson, 2004.
7. E. S. Gilreath, *Fundamental Concepts of Inorganic Chemistry*, International Student's Ed., Mcgraw-Hill Kogakusha, Ltd, 1958.
8. G. Chatwal and M. S. Yadu, *Coordination Chemistry*, 1st Ed., Himalaya Publishing House, 1992.
9. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Ed., John Wiley & Sons, 2010.
10. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Ed., , John Wiley & Sons, 2008.
11. B. R. Puri, L. R. Sharma and K. C. Kalia, *Text Book of Inorganic Chemistry*, Edited by P. L. Soni, Sultan Chand & Sons, New Delhi, 1993.
12. W. D. Loveland, D. J. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, Wiley-VCH Verlag GmbH Co. KGaA, 2006.
13. Glasstone, *Source Book on Atomic Energy*, 3rd Ed., East West Press, 1997**.**
14. H. J. M. Bowen, Buttler and Tanner, *Chemical Applications of Radioisotopes*, 1969.
15. G. Friedlander, T. W. Kennedy, E. S. Macias and J. M. Miller, *Introduction of Nuclear and Radiochemistry*, 3rd Ed., John Wiley, 1981.
16. C. N. R. Rao and J. Gopalakrishan, *New Directions in Solid State Chemistry*, Cambridge University Press.
17. A. R. West, *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1984.
18. K. Chakrabarty, *Solid State Chemistry*, New Age Publishers, 1996.

Semester: VI
Course Name: Bioorganic and Heterocyclic Chemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Amino acids, peptides and proteins: Classification, structure and stereochemistry of amino acids, Zwitterions, Isoelectric point, Electrophoresis, Synthesis, ionic properties and reactions of α-amino acids, Classification of proteins, Peptide structure determination: End group analysis and Selective hydrolysis of peptides, Solid-phase peptide synthesis, Primary and secondary structures of proteins.

UNIT – II 12 hours
Nucleic acids: Components of nucleic acids, Nucleosides and nucleotides, Synthesis of Adenine, Guanine, Cytosine, Uracil and Thymine, Structure of polynucleotides, Ribonucleosides and Ribonucleotides, The double helical structure of DNA.
Lipids: Introduction to oils and fats, Common fatty acids present in oils and fats, Hydrogenation of fats and oils, Saponification value, Acid value, Iodine number.

UNIT – III 12 hours
Enzymes: Classification and characteristics of enzymes, Salient features of active site of enzymes, Mechanism of enzyme action (chymotrypsin), Factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Mechanism of action of carboxypeptidase, Specificity of enzyme action (including stereospecificity), Enzyme inhibitors and their importance, Mechanism of action of coenzymes.

UNIT – IV 12 hours
Heterocyclic compounds-I: Classification and nomenclature, Methods of formation of five membered heterocycles: Furan, Thiophene and Pyrrole, Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis, Aromatic characteristics of pyrrole, furan and thiophene, Chemical reactions, Mechanism of electrophilic substitution.
Six membered heterocycles, Methods of formation of pyridine and pyrimidine, Mechanism of nucleophilic substitution reactions in pyridine derivatives, Comparison of basicity of pyridine, piperidine and pyrrole.

UNIT – V 12 hours
Heterocyclic compounds-II: Introduction to condensed five- and six-membered heterocycles, Preparation and reactions of indole, quinoline and isoquinoline, Fischer indole synthesis, Madelung synthesis, Skraup synthesis, Friedländer synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski synthesis, Pictet-Spengler reaction, Pomeranz-Fritsch reaction.

REFERENCES
1. T. L. Gilchrist, *Heterocyclic Chemistry*, 3rd Ed., Addison Wesley Longman Limited, 1997.
2. R. R. Gupta, M. Kumar and V. Gupta, *Heterocyclic Chemistry, Vol. I, II and III*, Springer Verlag, 1999.
3. J. A. Joule, K. Mills and G. F. Smith, *The Chemistry of Heterocycles*, 3rd Ed., Chapman and Hall, 1995.
4. *Comprehensive Heterocyclic Chemistry*, A.R. Katritzky and C.W. Rees (Eds.), Vol I-VIII, Ist Ed., Pergamon Press.

5. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Ed., 2010.
6. I. L. Finar, *Organic Chemistry*, Vol. I and II, 6th Ed., 2002.
7. D. L. Nelson and M. M. Cox, *Lehninger's Principles of Biochemistry*, 7th Ed., W. H. Freeman and Company, 2017.
8. J. M. Berg, J. L. Tymoczko, G. J. Gatto Jr. and L. Stryer, *Biochemistry*, 8th Ed., 2015.

Semester: VI
Course Name: Project/Dissertation
Course Code: **6 Credits (0-0-12)**

The students will identify a research problem and execute it under the supervision of a faculty member. They will learn literature survey, basic experimental and analytical techniques and carry out the research work. The research finding will be documented and a dissertation will be submitted. The students will deliver a power point presentation at the end of semester examination.

Semester: VI
Course Name: Spectroscopy and Computational Chemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Spectroscopy: Introduction: Electromagnetic radiation, Regions of the spectrum, Basic elements of practical spectroscopy, Lambert-Beer Law, Width and intensity of spectral lines, Statement of Born-Oppenheimer approximation.
Rotational spectroscopy: Diatomic molecules, Energy levels of a rigid rotor (semi-classical principles), Selection rules, Spectral intensity, Distribution using population distribution (Maxell- Boltzmann distribution), Rigid diatomic molecule, Non rigid rotator, Spectrum of non-rigid rotator, Polyatomic molecules, Determination of bond length, Isotope effect.

UNIT – II 12 hours
Vibrational spectroscopy: Infrared spectrum: Energy levels of simple harmonic oscillator, Selection rules, Pure vibrational spectrum, Intensity, Determination of force constant and qualitative relation of force constant and bond energies, Effect of anharmonic motion and isotope on the spectrum, Idea of vibrational frequencies of different functional groups, Vibration–rotation spectroscopy, P-branch and R-branch.
Raman spectroscopy: Concept of polarizability, Stokes and Anti-Stokes lines, Pure rotational and pure vibrational Raman spectra of diatomic molecules, Selection rules, Mutual Exclusion.

UNIT – III 12 hours
Electronic spectroscopy: The characteristics of electronic transitions, Electronic spectroscopy of atoms, Term symbol, Photoelectron spectroscopy, Electronic spectroscopy of molecules, Selection rules, Vibrational structure and Franck-Condon principle, Franck-Condon factor, Concept of HOMO-LUMO transitions, Simple Dissociation energy, Pre-dissociation, Quantum yield and radiative processes, Fluorescence and phosphorescence, Jablonski diagram, Internal conversion and intersystem crossing.

UNIT – IV 12 hours
Photochemistry: Generation of excited states, Singlet and triplet states, Spin-orbit coupling, Kinetics of photophysical and photochemical processes, Timescales, The primary quantum yield, Mechanism of decay of excited singlet states, Quenching, Stern-Volmer equation and its applications, Flash photolysis, Laser flash photolysis, Lasers and their applications.

UNIT – V 12 hours
Computers in chemistry: General introduction to computers, Different components of a computer, Hardware and software, Conceptual background of theory, Computations and molecular modeling,Z-matrix, Potential energy surfaces and chemical properties, Cost and efficiency, algorithms, Elementary ideas of molecular mechanics and force fields, Parameterization, Potential energy functional forms, Conceptual ideas of Molecular orbital methods, Concept of equilibrium structures, Transition state structures and harmonic frequency calculations, Born-Oppenheimer approximation, Awareness of computational chemistry software, Introduction to computer languages, Programming and operating systems.

REFERENCES

1. P. W. Atkins and J. de Paula, *The Elements of Physical Chemistry*, Oxford, 10th Ed., 2014.
2. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Co., 47th Ed., 2017
3. C. Banwell and E. McCash, *An Introduction to Molecular Spectroscopy*, McGraw Hills, 4th Ed., 1994.
4. C. Banwell, C. McCash and H. Chaudhury, *Fundamentals of Molecular Spectroscopy,* McGraw Hill Education, 4th Ed., 2013.
5. J. Michael Hollas, *Modern Spectroscopy*, Wiley, 4th Ed., 2004.
6. K. K. Rohatgi-Mukerjee, *Fundamentals of Photochemistry*, Wiley Eastern Ltd., 1986.
7. C. J. Cramer, *Essentials of Computational Chemistry*, Wiley-Blackwell, 2nd Ed., 2004.
8. F. Jensen, *Introduction to Computational Chemistry*, Wiley, 2nd Ed., 2007.
9. On-line manual of *Gaussian 16* and *GAMESS.* www.gaussian.com and www.msg.ameslab.gov/gamess
10. T. Engel and P. Reid, *Physical Chemistry*, Pearson, 2nd Ed., 2010.

Semester: VI
Course Name: Applied Chemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Polymers: Monomers and their functionality, Classification, Degree of polymerization, Type of polymerization, Addition and condensation polymerization, Mechanism of free radical, cationic, anionic and Ziegler-Natta polymerizations, Stereochemistry of polymer, Thermo- and thermosetting plastics, Preparation, properties and uses of Polythene, Polystyrene, PVC, Phenol-formaldehydes, Nylons, Kevlar, Terylene, Rubber: natural and synthetic rubbers, Silicone rubber.

UNIT – II **12 hours**

Dyes and paints: Classification of dyes, Synthetic dyes: Methyl orange, Congo red, Malachite green, Crystal violet, Primary constituents of a paint, Binders and solvents for paints, Oil based paints, Latex paints, Constituents of varnishes.

Soaps and detergents: Soap action, Raw materials for soaps, Classification and manufacture of soaps, Batch process, Continuous process, Difference between soap and detergent, Active ingredients in detergents, Anionic surfactant, Cationic surfactant, Amphoteric surfactant and Nonionic surfactant.

UNIT – III **12 hours**

Food additives: Food additives, Definition, Classification, Functions, Artificial sweeteners, Food flavors, Food colour, Acidulants, Antioxidants, Alkalies, Edible emulsifiers and edible foaming agents, Baking powder, Yeast, Sequesterants, Taste enhancers, Uses and abuses of these substances in food beverages.

Food preservation and processing: Food deterioration, Methods of preservation and processing, Food preservatives, Methods of preservation, Packaging of foods.

UNIT – IV **12 hours**

Cement: Type of cements, Raw material for manufacture, Manufacture of Portland cement, Manufacturing processes, Dry process, Wet process, Setting of cement, Hydrolysis, Hydration, Properties of cement, Role of gypsum in cement, Special type cements, High alumina cement, White cement, Mortar, Concrete and RCC, Curing and decay of concrete.

Glass: Physical and chemical properties of glass, Raw materials, Manufacture of glass by pot and tank furnaces, Types of glass, Tempered glass, Laminated glass, Water glass, Optical glass, Borosilicate glass, Lead glass, Safety glass, Fibre glass, Insulating glass.

UNIT – V **12 hours**

Fertilizers: Plant nutrients and its role, Classification of fertilizers, Properties of fertilizers, Nitrogenous fertilizers and its manufacture: Ammonium nitrate, Ammonium sulphate, Urea, Calcium cyanamide, Manufacture of phosphate fertilizer: Normal super phosphate, Triple super phosphate, Mono-ammonium phosphate, Diammonium phosphate, Potassium fertilizer, NPK fertilizer, Bio-fertilizers, Formulation and utilization,

Pesticides and insecticides: Classification of pesticides with examples and their modes of action, Organic and inorganic pesticides, Biopesticides, Impact of pesticides on soil, plants and environment.

REFERENCES

1. F. W. Billmeyer, *Textbook of Polymer Science*, John Wiley & Sons, Inc, 3rd Ed., 2007.
2. V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, *Polymer Science*, New Age International (P) Ltd. Pub, 2nd Ed., 2015.
3. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Ed., 2010.
4. G. N. Pandey, *Text Book of Chemical Technology*, Vol. 1 and 2, Vikas Publishing House, Pvt. Ltd, 1999.
5. E. Stocchi: *Industrial Chemistry, Vol-I*, Ellis Horwood Ltd. UK, 1990.
6. R. M. Felder and R. W. Rousseau, *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi, 3rd Ed., 2014.
7. M. Swaminathan, *Advanced Text Book on Food and Nutrition*, Volumes 1 and 2, Printing and Publishing CO., Ltd., 1993.
8. P. C. Jain and M. Jain, *Engineering Chemistry*, 16th Ed., Dhanpat Rai and Sons, Delhi, 2013.
9. T. P. Coultate, *Food – The Chemistry of its components*. Royal Society of Chemistry London, 2009.
10. M. Swaminathan, *Text Book on Food chemistry*, Printing and Publishing CO., Ltd., Bangalore. 1993.
11. M. F. Ali, B. M. El Ali and J. G. Speight, *Handbook of Industrial Chemistry: Organic Chemicals*, McGraw-Hill Education, 2005.
12. B. K. Sharma and H. Gaur, *Industrial Chemistry*, 16th Edition, Goel Publishing House, Meerut, 2011.

Semester: VII
Course Name: Bonding Theories and Inorganic Reaction Mechanisms
Course Code: **4 Credits (3-1-0)**

UNIT – I **14 hours**
Stereochemistry and bonding in main group compounds: VSEPR model, Bent rule, Energetics of hybridization, Structure and hybridization, *dπ–pπ* bonds, Structure and bonding in condensed phosphates, Catenation and heterocatenation, Heterocyclic ring system: P-N compounds, Cyclophosphazenes and cyclophosphazanes, S-N ring compounds S_4N_4, (SN)x, Homocyclic rings of S, Se and Te, Chemistry of silicon: Silanes, Higher silanes, Multiple bonded systems, Disilanes, Silicon nitrides, Siloxanes and silicates, Chemistry of boron, Boron cage compounds: Closo, Nido, Arachno, Carboranes, Borazines and boron nitrides, Cage compounds of S and P.

UNIT – II **12 hours**
Bonding theories-I: VB Theory and its application to H_2, Variation and LCAO methods, Molecular orbital theory, MO energy level diagrams for octahedral, tetrahedral and square planar complexes, Electron pair wave function, Hybrid orbitals, Localized and delocalized MO, σ, π, δ bonds, Nephelauxetic effect–angular overlap model, Polyatomic molecules, Electron deficient and hypervalent molecules.

UNIT – III **12 hours**
Bonding theories-II: The concept of a ligand field, Qualitative demonstration of ligand field effect, The physical properties affected by ligand field theory (thermochemical properties and geometric distortion), Spectral properties, Magnetic properties, Quantitative basis of crystal fields: Crystal field theory, Splitting of *d*-orbitals under various geometries, Factors affecting splitting–CFSE, Evidences for CFSE: Structural and thermodynamic effects, Spectrochemical series, Jahn-Teller distortion, Limitations of CFT, Effect of V_{oct} on the *d* wave functions, Evaluation of Δ.

UNIT – IV **10 hours**
Inorganic reaction mechanism-I: Energy profile of a reaction, Reactivity of metal complex, Inert and labile complexes, A-, D- and I-mechanisms for metal complexes, Kinetics of octahedral substitution, Acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Direct and indirect evidences in favour of conjugate mechanism, Anation reactions, Reactions without metal ligand bond cleavage.

UNIT – V **12 hours**
Inorganic reaction mechanism-II: Trans effect, Theories of trans effect, Mechanism of trans effect, Substitution reactions in octahedral complexes: Basic concepts of dissociation, Association and SN_1CB mechanism, Substitution reactions in square planar complexes, Kinetics of substitution reactions in square planar complexes, Brief outline of thermodynamic and kinetic stabilities of metal complexes, Stepwise and overall stability constants, Factors affecting the stability of complexes, Electron transfer reactions, Inner sphere, Outer sphere, Cross reactions and Marcus-Hush theory, Factors affecting the rates of outer sphere electron transfer reactions, Redox reactions, Non-complementary reactions.

REFERENCES

1. G. Wulfsberg, *Inorganic Chemistry*, Viva Books, 2016.
2. R. K. Sharma, *Inorganic Reaction Mechanisms*, Discovery Publishing House, 2011.

3. F. Basolo and R. G. Pearson, *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution*, 2nd Ed., John Wiley & Sons, 1967.
4. R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, 3rd Ed., OUP USA, 2007.
5. J. J. Li, *Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications*, 5th Ed., Springer.
6. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, Oxford University Press, 2006.
7. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Ed., Pearson, 2004.
8. G. Chatwal and M. S. Yadu, *Coordination Chemistry*, 1st Ed., Himalaya Publishing House, 1992.
9. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Ed., John Wiley & Sons, 2010.
10. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Ed., , John Wiley & Sons, 2008.
11. B. R. Puri, L. R. Sharma and K. C. Kalia, *Text Book of Inorganic Chemistry*, Edited by P. L. Soni, Sultan Chand & Sons, New Delhi, 1993.
12. W. D. Loveland, D. J. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, Wiley-VCH Verlag GmbH Co. KGaA, 2006.

Semester: VII
Course Name: Organic Reaction Mechanism and Stereochemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Structure and bonding: Bonding, Atomic and molecular orbitals, Hybridization, Electronic structure of molecules, Electronegativity, Dipole moment, Inductive and field effects, Bond distance, angle and energies, Cross conjugation, Resonance, Hyperconjugation, Steric inhibition of resonance, Tautomerism, Hydrogen bonding, Acids and Bases, Factors affecting the strength of acids and bases.

Aromaticity: Huckel's theory of aromaticity, Aromatic, antiaromatic and homoaromatic systems, Cyclopentadienyl anion and cation, MO description, Mobius twist and aromaticity, Heterocyclic aromatic systems, Aromaticity of annulenes and heteroannulenes, Fullerenes and fused ring systems.

UNIT – II **12 hours**

Reactive intermediates: Carbocation, carbanion, radicals, carbenes and nitrenes: Generation, geometry, stability and reactivity, Nucleophilicity, Heteroatom nucleophiles, Solvent effects, Alkene nucleophiles, α-Effect, Ambident nucleophiles: Thiocyanate, cyanide, nitrite and nitronium ions, Enolate ions, Allyl anions, Electrophilicity: Trigonal electrophiles, Tetrahedral electrophiles, Hard and soft electrophiles, Ambient electrophiles: Aromatic and aliphatic electrophiles.

Mechanistic aspects: Transition state theory, Intermediate, Transition state, Reaction coordinate diagram, Linear free energy relationships, Quantitative correlation of substituent effects on reactivity, Hammett and Taft equations, Microscopic reversibility, Basic mechanistic concepts like Kinetic versus thermodynamic control, Hammond postulate, Curtin-Hammett principle, Isotope effects, Cross over experiments.

UNIT – III **12 hours**

Stereochemistry: Optical activity and chirality, Stereochemistry of molecules with more than one asymmetric carbon (up to five), Homotopic and heterotopic ligands and faces, Heterotopicity, Enantiotopic and diastereotopic atoms, groups and faces, Stereotopic ligands and NMR spectroscopy, Prochiral centers: Chiral methyl, phosphate, sulphate and thiophosphate groups, Chirality of molecules devoid of chiral centers: Biphenyls, allenes, spiranes, molecules with planar chirality.

UNIT – IV **12 hours**

Conformational analysis: Conformational analysis of acyclic and cyclic compounds, Effect of conformation on reactivity in acyclic compounds and cyclohexanes: Stereoelectronic and steric factors, Oxidation of cyclohexanol, Esterification of cyclohexane carboxylic acid, Solvolysis of tosylates, E2 and *cis* eliminations, Formation and cleavage of epoxide ring, Neighboring group participation, Molecular rearrangements.

Conformation of cyclohexene and cyclohexanone, Conformation and stereochemistry of *cis*- and *trans*-decalins and 9-methyl decalin, Conformation of perhydrophenanthrene and perhydroanthracene.

UNIT – V **12 hours**

Asymmetric synthesis: Principles of asymmetric synthesis, Stereospecific and stereoselective reactions, Enantioselectivity and diastereoselectivity, Energetic considerations, Strategies for asymmetric synthesis, Analytical methods for determining enantiomeric excess, Resolving agents and resolution of racemic compounds having common functional groups such as alcohol, amine and acid, Sharpless epoxidation, symmetric dihydroxylation, asymmetric Diels-Alder reactions, Chiral borane reagents, Asymmetric reductions of prochiral carbonyl compounds and olefins.

REFERENCES

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6th Ed., Wiley, New Jersey, 2007.
2. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry: Part A: Structure and Mechanisms*, 5th Ed., Springer, New York, 2007.
3. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry: Part B: Reactions and Syntheses*: 5th Ed., Springer, New York, 2007.
4. R. Bruckner, *Organic Mechanisms*, Ed., M. Harmata, Springer, Berlin, 2010.
5. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford, 2001.
6. M. B. Smith, *Organic Synthesis*, 2nd Ed., McGraw-Hill, New Delhi, 2004.
7. F. A. Carey, *Organic Chemistry*, McGraw-Hill, New Delhi, 2000.
8. J. McMurry, *Organic Chemistry*, 5th Ed., Brooks/Cole, New York, 2000.
9. J. J. Li, Ed., *Name Reactions for Homologations*, Part II, Wiley, New Jersey, 2009.
10. C. J. Moody and G. H. Whitham, *Reactive intermediates*, Oxford Chemistry Primers, 1992.
11. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3rd Ed. CRC press, New York, 2012.
12. P. Sykes, *A guidebook to Mechanism in Organic Chemistry*, 6th Ed. Lingman Scientific & Technical, New York, 1986.
13. E. L. Eliel and S. H. Wilen, *Stereochemistry of Organic Compounds*, Wiley, New York, 2008.
14. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, 2nd Ed., New Age International, 2002.
15. P. S. Kalsi, *Stereochemistry: Conformation and Mechanism*, 9th Ed., New Age International, 2009.
16. J. D. Morrison, *Asymmetric Synthesis*, Vol 1-5, Academic press, 1983.
17. *Comprehensive Asymmetric Catalysis,* E. N. Jacobsen, A. Pfaltz, H. Yamamoto, Eds., Springer, 2000.
18. R. Noyori, *Asymmetric Catalysis in Organic synthesis*, Wiley-New York, 1994.
19. I. Ojima, *Catalytic Asymmetric Synthesis*, VCH-NY, Pergamon, 1998.
20. *Methods for the Asymmetric Synthesis of Complex Organic Molecules*, D. J. O'Leary, Lecture Notes 2001.
21. H. B. Kagan, *Aymmetric Synthesis*, 1st Ed., Thieme Medical Publishers, 2003.

Semester: VII
Course Name: Preparation of Inorganic Complexes and Analysis Lab
Course Code: 3 Credits (0-0-6)

PART A: Preparation of inorganic complexes (8-10 complexes)

1. $[VO(acac)_2]$
2. $[Mn(acac)_3]$
3. $[Co(en)_2(C_2O_4)]Cl.\ H_2O$
4. $[Co(NH_3)_5(NO_2)](NO_2)_2$
5. *Cis*- and *trans*- $[Co(en)_2Cl_2]Cl$
6. $Na[Cr(NH_3)(NCS)_4]$
7. $[Ni(acac)_2]$
8. $[Co(Py)_2Cl_2]$
9. $[Ni(NH_3)_6]Cl_2$
10. $[Co(NH_3)_6]\ [Co(NO_2)_6]$
11. *Cis*- $[Co(trien)(NO_2)_2]Cl.H_2O$
12. Pressian Blue,
13. Turnbull's Blue.

PART B: Analysis

1. Quantitative analysis of metals in complexes by Gravimetric/Volumetric techniques.
2. Structural investigation by I.R., Electronic spectra, Elemental analysis, UV-Visible spectroscopy and magnetic susceptibility measurements.

REFERENCES

1. J. Bassett, *Vogel's textbook of quantitative inorganic analysis, including elementary instrumental analysis*, 4th Ed., London, New York, Longman, 1978.
2. G. H. Jeffery, J. Basset, J. Mendham and R. C. Denny, *Vogel's Textbook of Quantitative Chemical Analysis*, 5th Ed.
3. G. Svehla and B. Sivasankar, *Vogel's Qualitative Inorganic Analysis*, 7th Ed., 2012.
4. G. R. Chatwal, *Instrumental Methods for Chemical Analysis*, 5th Ed., Himalaya Publications, India.
5. A.O. Thomas, *Practical Chemistry*, Scientific Book Centre, Cannanore, 2003.
6. J. Mendham, R. C. Denny, J. D. Barnes and M. J. K. Thomas, *Vogel's Text Book of Quantitative Chemical Analysis*, 6th Ed., Prentice Hall.
7. W. L. Jolly, *Synthesis & Characterization of Inorganic Compounds*, Prentice Hall. Vol-83 (6), 1971.
8. In-house laboratory manual with experimental procedures and relevant information.

Semester: VII
Course Name: Organic Preparation and Qualitative Analysis Lab
Course Code: 3 Credits (0-0-6)

PART A: Organic single stage preparation: 6-8 Experiments
Reactions Involved: Condensation, Oxidation, Nitration, Acetylation, Bromination, Diazotization-coupling and Rearrangement.

Conventional Experiments
1. Preparation of chalcone from acetophenone and benzaldehyde (Condensation)
2. Preparation of *p*-benzoquinone from hydroquinone (Oxidation)
3. Preparation of *m*-dinitrobenzene from nitrobenzene (Nitration)
4. Glucose pentaacetate from glucose (Acetylation)
5. 2,4,6-Tribromoaniline from aniline (Bromination)
6. Preparation of 1-phenyl-azo-2-naphthol from aniline and β-naphthol (Diazotization-coupling)
7. Nitrostyrene from benzaldehyde (Henry reaction)
8. Preparation of benzidine from hydrazobenzene (Rearrangement)

Green Synthesis
2. Three component, solvent-free synthesis of dihydropyrimidinone
3. Preparation of 1,1-bis-2-naphthol (Radical coupling)
4. Clay-catalyzed solid state synthesis of 7-hydroxy-4-methylcoumarin

PART B. Separation and qualitative analysis of an organic mixture containing two components: 4-6 Mixtures
Pilot separation, Bulk separation, Identification of functional groups, Elements present (N, S and halogens), Nature of the compounds *(aromatic/aliphatic, saturated/unsaturated),* Preparation of derivatives and determinations of physical constants (mp/bp).

The following kinds of organic compounds will be given for analysis.
1. Carboxylic acids and Dicarboxylic acids
2. Phenols and Naphthols
3. Amines (primary, secondary and tertiary)
4. Amides, Diamides, Anilides, Nitro compounds
5. Esters
6. Aldehydes and Ketones
7. Aromatic halogen compounds
8. Hydrocarbons
9. Carbohydrates

REFERENCES

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry,* 5th Ed., Pearson, 2012.
2. In-house laboratory manual with experimental procedures and relevant information.

Semester: VII
Course Name: Seminar
Course Code: **2 Credits (0-0-4)**

As part of this interactive course mentored by a faculty, the learners will be required to present the key research questions addressed, experimental design and major results from any recent publication in a reputed peer reviewed journal on any aspect of Chemistry – Organic, inorganic, physical, analytical or inter-disciplinary chemistry. They also are encouraged to technically critique the published article. The students will deliver a power point presentation at the end of semester examination.

Semester: VII
Course Name: Quantum Chemistry and Chemical Dynamics
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Basics of quantum mechanics: Postulates of quantum mechanics, Wave–particle duality, Uncertainty Principle, Operators algebra and commutation relations, Time dependent and independent Schrödinger equation, Particle in a box, Degeneracy, Tunneling, Particle in a ring, Delta function, Concept of angular momentum in quantum mechanics, Angular momentum operators and ladder operators, Harmonic oscillator, Rigid rotator and the hydrogen atom, Schrodinger equation for hydrogen atoms, Polar coordinates, Separations of variables and their solution (without derivation except for φ equation), Emergence of different quantum numbers and their significance, Shape and size of atomic orbitals.

UNIT – II 12 hours
Approximation methods: Methods of obtaining approximate solution to the time independent Schrödinger equation**,** Variational theory, Perturbation theory (non-degenerate) and their applications to simple problems, Anti-symmetry and exclusion Principle, Spin of electron, Terms symbols and spectroscopic states, Born – Oppenheimer approximation, Hydrogen molecule ion and hydrogen molecule Hamiltonian.

UNIT – III 12 hours
Applications of quantum mechanics: VB treatments of the hydrogen molecule, Concept of Coulomb integral, Exchange integral and Overlap integral, and their role in chemical binding, LCAO – MO, MO of homonuclear diatomic molecules and heteronuclear diatomic molecules (HF and CO), Hückel π-electron theory and its applications to conjugated systems, Hybridization, Basic idea of self-consistent field method.

UNIT – IV 12 hours
Chemical Dynamics-I: Determination of Rate laws, Arrhenius equations, Temperature dependence of reaction rate, Theory of absolute reaction rate: Thermodynamic and statistical mechanical approach, Evaluating probability factor, Consecutive, Opposing and Parallel reactions, Thermal and Photochemical reaction between H_2 and Br_2, Photochemical reaction between H_2 and Cl_2, decomposition of ethane, Belousov-Zhabotinsky reaction, Autocatalysis reaction.

UNIT – V 12 hours
Chemical dynamics-II: General features of fast reaction, Study of kinetics by Plug Flow and Stopped Flow techniques, Potential energy surface, Reaction coordinates and paths, Unimolecular reaction: Lindeman, Hinshelwood mechanism, RRK and RRKM theories.

REFERENCES

1. I. N. Levine, *Quantum Chemistry*, Pearson, 7th Ed., 2013.
2. N. S. Ostlund and A. Szabo, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover Publications, 1996.
3. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach*, Viva Student Ed., 2011.
4. D. A. McQuarrie, *Quantum Chemistry,* Viva Student Ed., 2014.
5. R. K. Prasad, *Quantum Chemistry*, New Age International Publishers Ltd., New Delhi, 4th Ed., 2014.

6. A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw Hill, 4^{th} Ed., 1998.
7. P. W. Atkins and R. Friedman, *Molecular Quantum Mechanics*, Oxford University Press, 5^{th} Ed., 2012.
8. J. P. Lowe and K. A. Peterson, *Quantum Chemistry*, Academic Press, 3^{rd} Ed., 2005.
9. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Co., 47^{th} Ed., 2017.
10. P. W. Atkins and J. de Paula, *The Elements of Physical Chemistry*, Oxford University Press,, 10^{th} Ed., 2014.
11. K. J. Laidler, *Chemical Kinetics*, McGraw Hill, New York, 3^{rd} Ed., 2003.

Semester: VII
Course Name: Analytical Chemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**
Separation techniques I: Ion exchange resins and their exchange capacities, Principle and simple applications of ion exchange separation, Chromatographic separations: Thin layer, Paper and Column chromatographic techniques and their simple applications, Types of adsorbents, R_f-values and their significance, Principle, Experimental techniques.

UNIT – II **12 hours**
Separation techniques II: Instrumentation and applications of Gas chromatography (GC) and High Pressure Liquid Chromatography (HPLC), GC-MS, LC-MS, Electrophoresis: Electrophoretic mobility, Eletroosmotic mobility, Instrumentation, Capillary electrophoresis methods. Isoelectric focusing.

UNIT – III **12 hours**
Electroanalytical methods I: 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 pKa values, Principle and applications of Electro gravimetry and coulometric analysis.|

UNIT – IV **12 hours**
Electroanalytical methods II: Polarography and cyclic voltammetry: Introduction, Instrumentation, Ilkovic equation and its verification, Derivation of wave equation, Determination of half wave potential, Qualitative and quantitative applications, Amperometry: Basic principles, instrumentation, nature of titration curves and analytical applications.

UNIT – V **12 hours**
Thermo analytical methods: Principle of thermo gravimetry, Differential thermal analysis, Differential scanning calorimetry, Instrumentation for TGA, DTA and DSC, Characteristics of TGA and DTA curves, Factors affecting TGA and DTA curves, Applications: TGA of calcium oxalate monohydrate, DTA of calcium acetate monohydrate, Determination of purity of pharmaceuticals by DSC.

REFERENCES

1. J. Mendham, R. C. Denney, J. D. Barnes and M. J. K. Thomas, *Vogel's Quantitative Chemical Analysis*, 6^{th} Ed., Pearson, 2009.
2. H. H. Willard, L. L. Merritt Jr., J. A. Dean and F. A. Settle Jr., *Instrumental Methods of Analysis*, 7^{th} Ed., Wardsworth Publishing Company, 1988.
3. G. D. Christian, *Analytical Chemistry*, 6^{th} Ed., John Wiley & Sons, New York, 2004.
4. D. C. Harris, *Exploring Chemical Analysis*, 9^{th} Ed., New York, W.H. Freeman, 2016.
5. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, 3^{rd} Ed., New Age International Publisher, 2008.
6. D. A. Skoog, F. J. Holler and S. R. Crouch, *Principles of Instrumental Analysis*, 7^{th} Ed., 2006.
7. O. Mikes, *Mikes Laboratory Hand Book of Chromatographic and Allied Methods (Elles Harwood Series on Analytical Chemistry)*, John Wiley & Sons, 1979.

Semester: VIII
Course Name: Group Theory, Transition Metal Chemistry and Photochemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Symmetry and group theory in chemistry: The concept of group, Sub-group, Point Symmetry group, Symmetry elements and Symmetry operations, Assignment of point groups to inorganic molecules, Some general rules for multiplications of symmetry operations, Multiplication tables for water and ammonia, Representations (matrices, matrix representation C_{2v} and C_{3v} point groups irreducible representations), Schonfilies symbols, Conjugacy relation and classes, Character and character tables for C_{2v} and C_{3v} point groups, The great orthogonality theorem (without derivation), Application of group theory to chemical bonding (hybrid orbitals for sigma bonding in different geometries and hybrid orbitals for π-bonding), Symmetries of molecular orbitals in BF_3, C_2H_4 and H_2O molecule.

UNIT – II 12 hours

Electronic spectra of transition metal complexes-II: Important features of transition metal electronic spectra-Band intensities, Band energies, Band width and sets, Group theoretical approach to selection rules, Effect of distortion and spin-orbit coupling on spectra (*3d*-, *4d*- and *5d*-transition series complexes), Spectrochemical and nephelauxetic series, Charge transfer spectra, Spectroscopic ground state, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1 to d^9 systems), Calculations of D_q, B and beta parameters, Jahn-teller effect, Electronic spectra of $[Ru(bipy)_3]^{2+}$.

UNIT –III 12 hours

Reagents in Inorganic Chemistry: Chelation, Factors determining the stability of chelates (effect of ring size, oxidation state of the metal, coordination number of the metal), Use of the following reagents in analytical chemistry and chemotherapy: Grignard's reagent, Tollen's reagent, Lucas' reagent, Fenton's reagent, Collman's reagent, Dimethylglyoxime, EDTA, 8-Hydroxyquinoline, 1,10-Phenanthroline, Thiosemicarbazones, Diathiazone.

UNIT – IV 12 hours

Principles and charge transfer of photochemistry: Absorption, Excitation, Photochemical laws, Quantum yield, Absorption and emission for complexes with different ground state/excited state for ML_6 complexes, Potential energy function and energy levels for ML_6complexes, Photolysis rules, Flash photolysis, Stopped flow techniques. Frank-Codon principle, Photochemical stages – Primary and secondary processes, Jablonski diagram for photochemical process.

Charge transfer photochemistry: Introduction, charge transfer absorption spectra, types of charge transfer excitations and their energy level scheme for charge transfer excitations, Types of reactions observed by charge transfer metal complexes.

UNIT – V 12 hours

Ligand field photochemistry of transition metal complexes: Photochemistry of Cr(III) complexes: Photo-substitutions, Properties of ligand field excited states, Photo aquation reactions, Photolysis rule, Photoisomerization, Photo racimization, Photoanation reactions, sensitizer, Energy transfer process, Mechanism of photosensitization, Photo reactive excited state, The Doublet hypothesis, Role of quartet excited states, Photophysics and photochemistry of ruthenium-polypyridyl complexes, Photo redox properties of Ce(III)and Ce(IV) complexes, photochemistry of Cu(II) (1,3 diketone) complexe Ligand-field photochemistry of Compounds with metal-metal bonding, Reinecke's salt chemical actinometer.

REFERENCES

1. D. M. Bishop, *Group Theory and Chemistry*, Revised Ed., Dover Publications, 1993.
2. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Revised Ed., Wiley-Blackwell, 1990.
3. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill Inc.,US, 1962.
4. J. M. Hollas, Chapman and Hall, *Symmetry in Molecules*, London, 1972.
5. H. H. Jaffe and M. Orchin, *Symmetry in Chemistry*, Dover Publications, 2002.
6. D. C. Harris and M. D. Bertolucchi, *Symmetry and Spectroscopy: An introduction to Vibrational and Electronic spectroscopy*, Dover Publications, 1990.
7. K. V. Reddy, *Symmetry and Spectroscopy of Molecules*, New Age International, 2009.
8. K. Bansal, *Group Theory and Symmetry in Chemistry*, 1st Ed., Campus Books International, 2006.
9. S. F. A. Kettle, *Symmetry and Structure*, 2nd Ed., John Wiley and Sons, 1995.
10. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, Elsevier, Amsterdam, Oxford, New York, 1984.
11. I. B. Bersuker, *Electronic Structure and Properties of Transition Metal Compounds: Introduction to the Theory*, 2nd Ed., John Wiley & Sons, 2010.
12. A. W. Adamson and P. D. Fleischauer, *Concepts of Inorganic Photochemistry*, John Wiley & Sons, New York, 1975.
13. S. F. A. Kettle, *Physical Inorganic Chemistry-A Coordination Chemistry*, Academic Publishers, Oxford University Press, 1996.
14. J. Ferraudi, *Elements of Inorganic Photochemistry*, Wiley, New York, 1988.
15. D. Farrusseng, *Metal-Organic Frameworks*, Wiley, 2011.
16. L. R. Mac Gillivray, *Metal-Organic Frameworks: Design and Application*, Wiley, 2010.
17. B. Chen and G. Qian, *Metal-Organic Frameworks for Photonics Applications*, Springer, 2014.

Semester: VIII
Course Name: Group Theory and Spectroscopy
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Group theory: Symmetry elements and symmetry operation, Definition of group, Sub-group, Relation between order of a finite group and its sub-group, Classes, Point symmetry group, Symmetry classification of molecules with examples. Elements of group theory: Dipole moment and optical isomerism.

UNIT – II 12 hours
Application of group theory: Representation of groups by matrices, Character of the representation, Reducible and irreducible representations, The great orthogonality theorem (without proof) and its importance, Construction of character tables and their applications, Determination of IR/RAMAN active modes of molecular vibrations, Symmetry and molecular orbital theory.

UNIT – III 12 hours
Rotational spectroscopy: Classification of rotors, Diatomic and linear polyatomic molecules, Transition frequencies or wave numbers, Rotational energy levels of polyatomic molecules, Intensities, Centrifugal distortion, Symmetric rotor molecules, Stark effect in diatomic, linear and symmetric rotor molecules, Asymmetric rotor molecules, Spherical rotor molecules.
Rotational Raman spectroscopy: Theory of rotational Raman scattering, Rotational Raman spectra of diatomic and linear polyatomic molecules, Rotational Raman spectra of symmetric and asymmetric rotor molecules, Structure determination from rotational constants.

UNIT – IV 12 hours
Vibrational spectroscopy: Diatomic molecules, Infrared spectra, Raman spectra, Anharmonicity, Vibration–rotation spectroscopy and spectral branches, Polyatomic molecules, Normal modes and vibrations of polyatomic molecules. Group vibrations, Number of normal vibrations of each symmetry species, Vibrational selection rules for IR and RAMAN spectra, Exclusion principle, Anharmonicity and potential energy surfaces.

UNIT – V 12 hours
Electronic spectroscopy: Atomic spectroscopy, Electronic angular momentum, Term symbol, Photoelectron spectroscopy, Electronic spectroscopy of diatomic molecules, Franck-Condon principle, Selection rules, Walsh diagram and molecular geometry, The electronic spectra of polyatomic molecules, *d–d* transitions, Charge-transfer transitions, $\pi^* \leftarrow \pi$ and $\pi^* \leftarrow n$ transitions, Resonance Raman transitions and application, Radiative and non-radiative decay-internal conversion and intersystem crossing, Fluorescence and phosphorescence, Jablonski diagram, Principles of Laser and its applications.

REFERENCES

1. P. W. Atkins and J. de Paula, *The Elements of Physical Chemistry*, Oxford University Press, 10th Ed., 2014.
2. F. A. Cotton, *Chemical Applications of Group Theory*, Wiley, 3rd Ed., 2008.
3. D. C. Harris and M. D. Bertolucchi, *Symmetry and spectroscopy: An introduction to vibrational and electronic spectroscopy*, Dover Publications, New Ed., 1990.

4. D. M. Bishop, *Group Theory and Chemistry*, Dover Publications Inc.; New Ed., 1993.
5. C. Banwell and E. McCash, *An Introduction to Molecular Spectroscopy*, McGraw Hill college, 4^{th}Ed., 1994.
6. C. Banwell and C. McCash, H. Chaudhury, *Fundamentals of Molecular Spectroscopy,* McGraw Hill Education, 5^{th} Ed., 2013.
7. J. Michael Hollas, *Modern Spectroscopy*, Wiley, 4^{th} Ed., 2004.
8. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Co., 47^{th} Ed., 2017.
9. T. Engel and P. Reid, *Physical Chemistry*, Pearson, 2^{nd} Ed., 2010.

Semester: VIII

Course Name: Organic Synthesis and Chromatography Lab

Course Code: **3 Credits (0-0-6)**

PART A: Organic double stage preparation (4-6 experiments)

1. *p*-Bromoaniline from acetanilide (Bromination/Hydrolysis)
2. Aspirin from methyl salicylate (Hydrolysis/Acetylation)
3. *p*-Aminobenzoic acid from p-nitrotoluene (Oxidation/Reduction)
4. *m*-Nitroaniline from nitrobenzene (Nitration/Reduction)
6. *p*-Nitroacetanilide from aniline (Acetylation/Nitration)
7. *m*-Nitrophenol from m-dinitrobenzene (Reduction/Diazotization-coupling)
8. *p*-Toluenesulphonamide from toluene
9. Dichloramine-T from toluene

PART B: Extraction of natural products (any two)

1. Extraction of caffeine from tea leaves
2. Isolation of clove oil (eugenol and eugenol acetate) by steam distillation
3. Extraction of piperine from black pepper
4. Extraction of lycopene from tomatoes

PART C: Analysis of the given mixture by TLC and column chromatography separation (4-6 mixtures)

1. Monitoring reaction progress of PART A by TLC
2. Mixtures of compounds with a range of polarity difference will be given for separation

REFERENCE

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5th Ed., Pearson, 2012.
2. In-house laboratory manual with experimental procedures and relevant information.

Semester: VIII
Course Name: Thermodynamic, Kinetics and Spectroscopy Lab
Course Code: **3 Credits (0-0-6)**

PART A: Thermodynamics

1. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
2. Study the influence of ionic strength on the solubility of $CaSO_4$ and hence determine its thermodynamic solubility product and mean ionic activity.

Phase equilibrium

3. Determination of equilibrium constant of the reaction $KI + I_2 \rightleftharpoons KI_3$ by distribution method.
4. Determination of distribution coefficient of succinic acid between benzene and water.
5. Determination of critical solution temperature of binary system (Phenol-water) and the effect of addition of salt in it.
6. To construct the phase diagram for three component systems.
7. To construct the phase diagram for a two component system (eutectic point)

PART B: Kinetics

1. Determination of rate constant of saponification of ethyl acetate by NaOH.
2. Determination of the velocity constant of hydrolysis of an ester in micellar media.
3. Determination of the relative strength of two acids (hydrochloric acid and sulphuric acid) studying the hydrolysis of methyl acetate.
4. Determination of autocatalytic reaction between potassium permanganate and oxalic acid.
5. Investigate the adsorption of oxalic acid/acetic acid by activated charcoal and test the validity of Freundlich/Langmuir isotherms.

PART C: Spectroscopy

1. Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
2. Verification of Beer's law in case of a given colored solution.
3. Determination of Indicator constant (pK_{In}) of methyl red colometrically.

REFERENCES

1. A . Ghoshal, B. Mahapatra and A. K. Nad, *An Advanced Course in Practical Chemistry,* New Central Book Agency Pvt. Ltd., 3rd Ed., 2012.
2. B. P. Levitt, *Findley's Practical Physical Chemistry*, Longman Group Ltd., 9th Ed., 1973.
3. J. B. Yadav, *Advanced Practical Physical Chemistry*, Goel Publishing, 2014.
4. B. Viswanathan and P. S. Raghavan, *Practical Physical chemistry*, Viva Books Pvt. Ltd., 2005.
5. In-house laboratory manual with experimental procedures and relevant information.

Semester: VIII
Course Name: Organic Synthesis and Reaction Mechanism
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Aliphatic nucleophilic substitution: S_N1, S_N2, S_Ni and SET mechanisms, Reactivity, Structural and solvent effects, Stereochemical aspects, The neighboring group mechanism, Substitution in norbornyl and bridge-head systems, Substitution at benzylic, allylic and vinylic carbons, Substitution at sp^2 carbons, Alkylation and acylation of amines, Alkylation and acylation of active methylene compounds, Hydrolysis of esters, Claisen and Dieckmann condensation.

Aromatic nucleophilic substitution: S_NAr via Meisenheimer complex, Benzyne and $S_{RN}1$ mechanisms, Reactivity, Cine substitution, Chichibabin reaction.

Electrophilic substitution: S_E1, S_E2 and S_Ei Mechanisms, Aromatic electrophilic substitution via Wheland intermediates, Orientation and reactivity, Ortho effect, Substitution of H^+ versus ipsosubstitution, Individual reactions: Ar-Halogen, Ar-SO_3H and Ar-NO_2 bond formation, Diazonium coupling, Friedel-Crafts related reactions and Vilsmeier-Haack.

UNIT – II **12 hours**

Addition reactions: Addition to C-C multiple bonds, Electrophilic, nucleophilic and free radical addition, Mechanisms, Orientation and reactivity, Stereochemistry of addition reactions of alkenes: Bromine addition, Hydrogen bromide addition, Catalytic hydrogenation and Hydroboration-oxidation, 1,2 and 1,4-additions of organometallic reagents (Mg, R_2CuLi), Michael addition, Addition to C-heteroatom multiple bond.

Elimination reactions: E1, E2, and $E1_CB$ Mechanisms, Regioselectivity, Stereochemistry of elimination: Cyclic and acyclic systems, Bredt's rule, Pyrolytic elimination, Chugaev reaction, Hofmann degradation, Shapiro reaction, Cope elimination, Competition between substitution and elimination.

UNIT – III **12 hours**

Molecular rearrangements: Mechanism and stereochemical aspects of Pinacol-pinacolone, Demjanov, Wagner-Meerwein, Pummerer, Beckmann, Schmidt, Benzilbenzilic acid, Favorskii, Hofmann, Curtius, Lossen, Wolff, Fries, Baeyer-Villiger, Sommelet-Hauser, Stevens rearrangements, Problems on rearrangement.

UNIT – IV **12 hours**

Retrosynthetic analysis: Disconnection approach, Synthons and synthetic equivalents, Transform, Functional group interconversion, Umpolung, Chemo-, regio and stereoselectivities, One group disconnection: Alcohols and carbonyl compounds, Two group disconnections: 1,2-, 1,3-, 1,4-, 1,5-, and 1,6-difunctional compounds, Diels-Alder reactions, Robinson annulation, Michael addition, Retrosynthetic analysis of longifolene.

UNIT – V **12 hours**

Protecting groups in organic synthesis: Importance, Protection and deprotection of hydroxyl groups: MOM, MTM, SMOM and THP ethers, Silyl ethers (TMS, TES, TIPS, TBDMS and TBDPS ethers), Protection for 1,2- and 1,3-diols, Protection and deprotection of carbonyl compounds: Acyclic and cyclic acetals and ketals, monothio and dithioacetals and ketals, Monoprotection of dicarbonyl compounds, Protection of amines, Boc, Cbz, PMB, Bn, Ac, Bz and Ts. Common protecting groups for carboxylic acids and thiols.

REFERENCES

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6^{th} Ed., Wiley, New Jersey, 2007.
2. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry: Part A: Structure and Mechanisms*, 5^{th} Ed., Springer, New York, 2007.
3. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry: Part B: Reactions and Syntheses*: 5^{th} Ed., Springer, New York, 2007.
4. R. Bruckner, *Organic Mechanisms*, Ed., M. Harmata, Springer, Berlin, 2010.
5. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford, 2001.
6. M. B. Smith, *Organic Synthesis*, 2^{nd} Ed., McGraw-Hill, New Delhi, 2004.
7. F. A. Carey, *Organic Chemistry*, McGraw-Hill, New Delhi, 2000.
8. J. McMurry, *Organic Chemistry*, 5^{th} Ed., Brooks/Cole, New York, 2000.
9. J. J. Li, Ed., *Name Reactions for Homologations*, Part II, Wiley, New Jersey, 2009.
10. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2^{nd} Ed., Wiley, 2008.
11. S. Warren and P. Wyatt, *Organic Synthesis: Strategy and Control*, Wiley, 2007.
12. E. J. Corey and X.-M. Cheng, *The Logic of Chemical Synthesis*, Wiley, 1995.
13. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6^{th} Ed., Wiley, New Jersey, 2007.
14. P. G. M. Wuts and T. W. Greene, *Greene's Protective Groups in Organic Synthesis*, 4^{th} Ed., Wiley, 2006.
15. Philip J. Kocienski, *Protecting groups*, 3^{rd} Ed., Thieme, 2005.

Semester: VIII
Course Name: Organic Spectroscopy and Organometallics
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

UV-VIS spectroscopy: Woodward-Fieser rules, UV spectra of aromatic and heterocyclic compounds, Applications of UV-VIS spectroscopy in organic chemistry.
IR Spectroscopy: FT technique, Characteristic functional group absorptions, Factors influencing group frequencies, Hydrogen bonding, Overtones, Combination bands, Fermi Resonance, NIR spectroscopy.
Optical rotatory dispersion and circular dichroism: Introduction to theory and terminology, Cotton effect, ORD curves, Axial haloketone rule and its applications, Octant rule, Applications of ORD to determine absolute configuration of monocyclic ketones, Comparison between ORD and CD – their inter relationships.

UNIT – II 12 hours

NMR spectroscopy: ^{1}H-NMR: FT technique, Shielding, Chemical shift, Diamagnetic anisotropy, Integration, Exchangeable hydrogens, Chemical equivalence, Magnetic equivalence, Spin coupling, Non-first order spectra, Spin systems (AB, AX, AB_2, AX_2, AMX, ABX, ABC etc.), Geminal, Vicinal and Long range coupling, Coupling constants, Spin decoupling, Relaxations, Nuclear Overhauser effect, NMR shift reagents, Variable temperature ^{1}H-NMR, Coupling of proton with ^{13}C, ^{19}F, ^{31}P and ^{29}Si.
^{13}C-NMR: Proton-decoupled and off-resonance, Chemical shifts, DEPT (45, 90 and 135).
2D NMR: Introduction, HOMOCOSY, HETCOR, HMQC, HMBC, INADEQUATE and NOESY.

UNIT – III 12 hours

Mass spectrometry: Mass spectrometry, Principle, Basic instrumentation, Ionization techniques – EI, CI, FD and FAB, Fragmentation, Molecular ion peak, Base peak, Metastable ions, Isotopes, Nitrogen rule, McLafferty rearrangement, Retro Diels-Alder, Characteristic fragmentation patterns of hydrocarbons, ethers, alcohols, phenols, ketones, aldehydes, carboxylic acids, amides, HRMS, Introduction to ESI-MS and MALDI-TOF.

UNIT – IV 12 hours

Applications of spectroscopic techniques: Problems on the structural elucidation of organic compounds using UV, IR, NMR and Mass techniques.

UNIT – V 12 hours

Organometallic reagents: Organozinc and copper reagents: Preparation, Functionalized zinc and copper reagents, Synthetic applications, Gilman reagents, Reformatsky reaction, Simmons-Smith reaction, Grignard and organolithium reagents in organic synthesis, Organoboron reagents, Synthetic application of Sn and Si reagents, Wittig, Horner-Wadsworth-Emmons Reactions, Cross-coupling reactions (Suzuki, Heck), Ring closing metathesis.

REFERENCES

1. R. M. Silverstein and F. X. Webster, *Spectroscopic Identification of Organic Compounds*, 6th Ed., Wiley, 2004.
2. P. S. Kalsi, *Spectroscopy of Organic Compounds*, New Age International, 6th Ed., 2006.

3. W. Kemp, *Organic Spectroscopy*, Palgrave, 2008.
4. H. Friebolin, *Basic One and Two Dimensional NMR Spectroscopy*, 5th Ed., Wiley-VCH, 2010.
5. A. Upadhyay, K. Upadhyay and N. Nath, *Biophysical Chemistry – Principles and Techniques*, 4th Ed., Himalaya Publishing House, 2010.
6. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, *Instrumental Methods of Analysis*, 7th Ed., CBS Publishers & Distributors, 2004.
7. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*: *Part A: Structure and Mechanisms*, 5th Ed., Springer, New York, 2007.
8. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*: *Part B: Reactions and Syntheses*, 5th Ed., Springer, New York, 2007.
9. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford, 2001.
10. M. B. Smith, *Organic Synthesis*, 2nd Ed., McGraw-Hill, New Delhi, 2004.
11. F. A. Carey, *Organic Chemistry*, McGraw-Hill, New Delhi, 2000.
12. J. McMurry, *Organic Chemistry*, 5th Ed., Brooks/Cole, New York, 2000.

Semester: IX
Course Name: Thermodynamics and Electrochemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**
Chemical thermodynamics: Statistical interpretation of entropy, Residual entropy, Chemical potential.
Phase equilibrium: Gibbs energies of pure phases and allotropes, Phase equilibria of two component systems (simple eutectic systems) and three component system (acetic acid-chloroform-water system).
Ideal and non-ideal solutions: Properties of ideal and non-ideal systems, Excess functions for non-ideal solutions, Vapour pressure-composition and boiling point-composition of completely miscible binary solutions, Partial molar quantities, Determination of partial molar volume and enthalpy. Colligative properties of dilute solutions: Elevation of boiling point, depression of freezing point and Lowering of vapor pressure. (thermodynamic treatment).

UNIT – II **12 hours**
Statistical thermodynamics-I: Concept of distribution, Thermodynamic probability, Ensemble averaging, Canonical, Grand canonical and micro canonical ensembles, Micro and macro states, Types of statistics: Maxwell-Bolzmann, Bose-Einstein and Fermi-Dirac, Most probable distribution of these types of statistics, Comparison of three statistics, Stirling's approximation, Molecular partition function and its significance.

UNIT – III **12 hours**
Statistical thermodynamics-II: Factorization of molecular partition function, Partition function for: independent and distinguishable molecules as well as independent and indistinguishable particles, Evaluation of translational, rotational, vibrational and electronic partition function and calculation of thermodynamic properties, Chemical equilibria and equilibrium constant in terms of partition functions.

UNIT – IV **12 hours**
Electrochemistry-III: Debye-Huckel limiting law, Debye-Huckel-Onsagar treatment and its extension, Debye-Huckel-Jerum mode, Thermodynamics of electrified interfaces, Variation of interfacial tension with applied potential (Lippman equation), Variation of charge on electrode with potential (Determination of electrical capacitance of interface), Variation of surface tension with solution composition (Determination of surface excess), Structure of electrified interfaces: Helmholtz-Perrin, Guoy-Chapman, Stern models.

UNIT – IV **12 hours**
Electrochemistry-IV: Analogies between semiconductors and electrolytic solution, Structure of semi conductor-electrolyte interface, Diffuse charge region inside an intrinsic semiconductor (The Garrett-Brattain space).
Bioelectrochemistry, Threshold membrane phenomenon, Nernst-Planck equation, Electrocardiography.
Introduction to corrosion, Homogeneous theory, Types of corrosion, Corrosion monitoring and prevention methods.

REFERENCES

1. P. W. Atkins and J de Paula, *Physical Chemistry*, Oxford University Press, 10th Ed., 2014.

2. M. C. Gupta, *Statistical Thermodynamics*, John Wiley & Sons, 1st Ed., 1991.
3. D. A. McCurrie, *Statistical Mechanics,* Viva Student Ed., 2014.
4. J. O. M. Bockris and Amulya K. N. Reddy, *Modern Electrochemistry* – Vol – I & II, by, Plenum.
5. K. L. Kapoor, *Physical Chemistry*, McGraw Hill Education, Vol. 1, 2, 3 and 5, 2016
6. Donald A. McQuarrie and John D. Simon, *Physical Chemistry: A Molecular Approach*, Viva Student Ed., 2011.
7. R. P. Rastogi and R. R. Mishra, *Chemical Thermodynamics*, Vikas Publishing House Pvt. Ltd., 6th Ed., 2009.
8. S. Glasstone, *An Introduction to Electrochemistry*, Affiliated East-West Press Pvt. Ltd., New Delhi, 2006.
9. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, Vishal Publishing Co., 47th Ed., 2017.

Semester: IX
Course Name: Reagents, Photochemistry and Heterocyclic Chemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Oxidation reactions: Swern oxidation, HIO_4, $Pb(OAc)_4$, $Hg(OAC)_2$, $I_2/AgOAc$, Woodward and Prevost reactions, Sharpless asymmetric epoxidation and Peroxyacids, Ozone, PCC, PDC, Etards reagent, MnO_2, OsO_4, SeO_2, DDQ, RuO_4, Jones reagent, Copper chromite and Wacker's reagent ($PdCl_2$), Iodobenzenediacetate, IBX, Dess-Martin periodinane.
Reduction reactions: Metal hydrides $LiAlH_4$, $NaBH_4$, $Na(CN)BH_3$, $Zn(BH_4)_2$ and trialkyltin hydrides, DIBAL, Metals in acidic medium (alkali metals, tin and zinc), H_2/metal catalysts (hydrogenation), $SnCl_2$ and Lawessonn reagent, $TiCl_4$/Zn-Cu (McMurray reagent), Wilkinson's catalyst, Lindlar catalyst, BH_3/THF, 9-BBN and chiral boranes.

UNIT – II 12 hours
Pericyclic reactions: Definition, Electrocyclic reactions, Cycloaddition reactions, Sigmatropic reactions: Orbital symmetry, HOMO and LUMO orbitals, Stereochemical aspects, Frontier molecular orbital approach, Correlation diagram approach, Woodward-Hoffmann rules, Concepts of con and dis rotation, Cyclization of butadienes and 1,3,5-hexatrienes, Suprafacial and antarafacial additions, [2+2], [4+2] and other cycloadditions, Diels-Alder reactions, Stereospecificity, endoselectivity and regioselectivity, Dipolar and intramolecular cycloaddition reactions, [1,3], [1,5] and [2,3] sigmatropic reactions, Claisen, Cope and oxy-Cope rearrangements, Cheletropic reactions.

UNIT – III 12 hours
Organic photochemistry: Fundamental concepts, Jablonski diagram, Energy transfer, Characteristics of photoreactions, Photoreduction and photooxidation, Photoreactions of ketones, enones, Norrish type I and II reactions, Photoaddition of nitrenes, Photochemistry of alkenes, dienes and aromatic compounds, Photoinduced isomerization, Reactions of unactivated centers, Photolytic cycloadditions, Photolytic rearrangements: Di-pi methane and oxa di-pi methane rearrangements, Photo Fries rearrangement, Photosensitization, Photoadditions, Barton reaction, Paterno-Buchi reaction, Application of photochemical reactions in organic synthesis.

UNIT – IV 12 hours
Heterocyclic compounds: Nomenclature of heterocycles, Structure, preparation, properties and reactivity of furan, pyrrole, thiophene, pyridine, indole, quinoline, isoquinoline and their derivatives, Synthesis and reactivity of pyrazoles, imidazoles, oxazoles, pyridazines, pyrimidines and pyrazines.

UNIT – V 12 hours
Natural products chemistry: General methods of structural elucidation of alkaloids and terpenoids, Total synthesis and stereochemical aspects of Reserpine (Woodward), (-)-Lepenine (Fukuyama) and Chloestrol (Robinson), Biosynthesis of steroids.

REFERENCES

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6th Ed., Wiley, New Jersey, 2007.
2. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*: *Part A: Structure and Mechanisms*, 5th Ed., Springer, New York, 2007.

3. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*: *Part B: Reactions and Syntheses*: 5th Ed., Springer, New York, 2007.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford, 2001.
5. M. B. Smith, *Organic Synthesis*, 2nd Ed., McGraw-Hill, New Delhi, 2004.
6. F. A. Carey, *Organic Chemistry*, McGraw-Hill, New Delhi, 2000.
7. J. McMurry, *Organic Chemistry*, 5th Ed., Brooks/Cole, New York, 2000.
8. J. D. Coyle, *Introduction to Organic Photochemistry*, Wiley, 1986.
9. J. M. Coxon and B. Halton, *Organic Photochemistry*, 2nd Ed., Cambridge University Press, 1986.
10. I. L. Finar, *Organic Chemistry* Vol. 1, Pearson, 2009.
11. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4th Ed., Cambridge University Press, 2004.
12. I. Fleming, *Pericyclic Reactions*, Oxford University Press, 1998.
13. S. Sankararaman, *Pericyclic Reaction – A Text Book: Reactions, Applications and Theory*, Wiley, 2005.
14. J. Mann, R. S. Davidson, J. B. Hobbs, D.V. Banthrope and J. B. Harborne, *Natural Products: Their Chemistry and Biological Significance*, Harlow, Essex, England Longman Scientific & Technical, New York, Wiley, 1st Ed., 1994.
15. Atta-ur-Rahman M. I. Choudhary, *New Trends in Natural Product Chemistry*, 1998, Harwood Academic Publishers.
16. I. L. Finar, *Organic Chemistry*, Vol. II, 3rd Ed., 1964.

Semester: IX
Course Name: Inorganic Preparation, Analysis and Chromatography Lab
Course Code: 4 Credits (0-0-6)

PART A: Preparation of inorganic compounds (6-8 experiments)
Preparation of selective inorganic compounds and characterize them by the following techniques: Elemental analysis, molar conductance values, IR spectral interpretation, thermal analysis, Electronic spectra, and UV-Visible spectroscopy.
Selection can be made from the following:

1. Preparation of trans-dicholoro bis(ethylenediamine)cobalt(III) chloride.
2. Preparation of tris(ethylenediamine)nickel(II) chloride.
3. Preparation of tetraamminecarbonatocobalt(III) nitrate.
4. Preparation of pentaamminecholorocobalt(III) chloride.
5. Preparation and mangnetic moment of $Cu(acac)_2H_2O$.
6. Separation of optical isomer cis-$[Co(en)_2Cl_2]Cl$.
7. Ion exchange separation of oxidation state of vanadium.
8. Preparation of Fe(II)chloride (use it as Friedel-Craft chlorination source).
9. Preparation and use of Ferrocene.
10. Preparation of phosphine Ph_3P and its transition metal complexes.
11. Reaction of Cr(III) with a multidentate ligand: a kinetic experiment (visible spectra Cr-EDTA complex).
12. Preparation of Chromium(III) complexes, $[Cr(H_2O)_6]NO_3.3H_2O.[Cr(H_2O)]_4Cl_2]Cl.2H_2O$, $[Cr(en)_3]Cl_3.Cr(acac)_3$.

PART B: Gravimatric and volumetric analysis (2-3 analysis)
Vanadium, Nickel, Manganese, Aluminium, Chromium, Chloride (Volhard's method).

PART C: Separation by paper/TLC/column chromatography and estimations

1. Separation of Cobalt(II) and Nickel(II) on anion exchange column followed by estimation through EDTA titrations.
2. Separation of two Cobalt (III) complexes *viz* $[Co(NH_3)_6]Cl_3$ and $[Co(NH_3)_5Cl]Cl_2$ on silica column.
3. Determination of R_f value of cations of transition metal ions by paper and thin layer chromatography.

REFERENCES

1. G. H. Jeffery, J. Basset, J. Mendham and R. C. Denny, *Vogel's Textbook of Quantitative Chemical Analysis*, 5th Ed.
2. G. Svehla and B. Sivasankar, *Vogel's Qualitative Inorganic Analysis*, 7th Ed., 2012.
3. G. R. Chatwal, *Instrumental Methods for Chemical Analysis*, 5th Ed., Himalaya Publications, India.
4. In-house laboratory manual with experimental procedures and relevant information.

Semester: IX
Course Name: Electrochemistry and Computational Chemistry Lab
Course Code: 3 Credits (0-0-6)

PART A: Electrochemistry

1. Determination of the strength of strong and weak acids in a given mixture conductometrically.
2. Determination of the strength of strong and weak acids in a given mixture pH-metrically.
3. Determination of activity co-efficient of zinc ions in the solution of 0.002 M $ZnSO_4$ using Debye-Huckel's limiting law.
4. Determine the degree of hydrolysis and the hydrolysis constant of aniline hydrochloride by pH/potentiometry.
5. Titrate pure solutions of KCl, KBr and KI and their mixture with standard $AgNO_3$ solution potentiometrically.
6. Determination of the pK_a value of the given organic acid by pH measurement.
7. To determine the Ionization constant of a weak acid conductometrically.
8. Study the conductometric titration of strong acid *Vs* strong base.
9. Determination of the composition of a mixture of hydrochloric acid and oxalic acid conductometrically.
10. Determination of solubility product of a sparingly soluble salt in water by conductance measurement.
11. Determination of hydrolysis constant of aniline hydrochloride by conductance measurement.
12. Determination of the acid and base dissociation constant of an amino acid (glycine/histidine/cysteine) and hence the iso-electric point of the acid.
13. Determination of the molar conductivity of weak mono – basic acid over a given range of concentration.
14. Titration of HCl + Acetic acid + CuSO4 Vs. NaOH conductometrically.
15. pH-metric titration of o-Phosphoric acid Vs. NaOH.

PART B: Computational Chemistry

To run Computational Chemistry software (Gaussian 16, GAMESS, etc).

1. Determination of the strength of strong and weak acids in a given mixture conductometrically.
2. pH-metric titration of o-Phosphoric acid Vs. NaOH.
3. Finding minima and maxima (optimization and frequency calculations of equilibrium structures and transition states) of simple molecules.
4. Study of Intrinsic Reaction Coordinate (IRC) and PES scanning.
5. Electronic charge analysis (Mulliken, NBO, etc).
6. Conformational study of Ethane and Butane and hence to determine their potential energy surfaces.
7. Calculation of thermodynamic parameters, study of cis-trans isomerisation.
8. Study the equilibrium constants, rate constants and the effect of substitutions on such quantities.
9. Simple programming in FORTRAN (summation for array of data, factorization, iteration).

REFERENCES

1. A. Ghoshal, B. Mahapatra and A. K. Nad, *An Advanced Course in Practical Chemistry,* New Central Book Agency Pvt. Ltd., 3rd Ed., 2012.
2. J. B. Yadav, *Advanced Practical Physical Chemistry*, Goel Publishing, 2014.
3. B. Viswanathan and P. S. Raghavan, *Practical Physical chemistry*, Viva Books Pvt. Ltd., 2005.
4. C. J. Cramer, *Essentials of Computational Chemistry-Theories and Models*, John Wiley and Sons Ltd., 2nd Ed., 2004.
5. F. Jensen, *Introduction to Computational Chemistry*, John Wiley and Sons Ltd., 3rd Ed., 2017.
6. On-line manual of *Gaussian 16* and *GAMESS.* www.gaussian.com and www.msg.ameslab.gov/gamess
7. Arnold Robbins, Elbert Hannah and Linda Lamb, *Learning the vi and Vim Editors: Text Processing at Maximum Speed and Power*, O'Reilly Media, 7th Ed., 2009.
8. K. V. Raman, *Computers in Chemistry*, Tata McGraw Hill Education, 1st Ed., 2004.
9. V. Rajaraman, *Computer programming in C*, Prentice Hall, 1994.
10. S. A. Mollah, *Introduction to Numerical Analysis,* Books and Allied Pvt. Ltd., 3rd Ed., 2012.
11. William H. Press, Saul A. Teukolsky , William T. Vetterling and Brian P. Flannery, *Numerical Recipes in Fortran 90: The Art of Scientific Computing*, Cambridge University Press, 2nd Ed., 1996.
12. In-house laboratory manual with experimental procedures and relevant information.

Semester: IX
Course Name: Project Phase I
Course Code: 4 Credits (0-0-8)

The students will identify a research problem and execute it under the supervision of a faculty member. They will carry out literature survey and do the preliminary research work. The students will submit a one page abstract and give a power point presentation at the end of semester examination.

Semester: IX
Course Name: Bio-inorganic and Supramolecular Chemistry
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Basics of bioinorganic chemistry: Introduction to bioinorganic chemistry, bioinorganic elements (essential and trace) according to their action in biological system, Generation of concentration gradients (Na^+-K^+ pump), Nitrogen fixation(biological and chemical nitrogen fixation), DNA polymerization, Basics of biomineralisation, Metal ions present in biological systems, Uptake, Transport and storage of metal ions by organisms-Structure and functions of biological membranes, Molybdenum nitrogenase, Metals at the centre of photosynthesis, Primary processes in photosynthesis–Photosystems I and II, Excess and deficiency of some trace metals, Toxicity of metal ions (Hg, Pb and As).

UNIT – II 12 hours
Electron transfer in biology/metal ion storage and transport: Structure and properties of : haemoglobin, myoglobin, hemerythrin and hemocyanine, Synthetic oxygen carriers, Model systems: Blue copper proteins, Iron-sulfur proteins, Ferritin, Metallothioneins, Cerruloplasmin, Siderophores–Enterobactin, Transferin, Structure and function of metalloproteins in electron transport processes: Iron enzymes-Peroxidase, Catalase and cytochrome P-450, Copper enzymes-Superoxide dismutase, Vitamin B_{12} and B_{12} coenzymes, Zinc enzymes–Carboxypeptidase and carbonicanhydrase, Molybdenum oxotransferase enzymes–Xanthine oxidase.

UNIT – III 12 hours
Basics of supramolecular chemistry: Definition of supramolecular chemistry, Nature of binding interactions in supramolecular structures: Ion-ion, Ion-dipole, Dipole-dipole, H-bonding, Cation-*p*, Anion-*p*, *p-p*, and van der Waals interactions, Self-assembly, Macrocyclic and template effects, Host-guest interactions, Pre-organization and complimentarity, Lock and key analogy, Binding of cationic, Anionic, Ion pair and neutral guest molecules.

UNIT – IV 12 hours
Supramolecular chemistry and molecular recognition: Molecular recognition: Introduction to recognition, Information and complementarity, Molecular receptors-Design principles, Spherical recognition-Cryptates of metal cations, Tetrahedral recognition by macrocyclic cryptands, Recognition of ammonium ions and related substrates, Recognition of neutral molecules, Recognition of anionic substrates (anionic coordination), Synthesis and structure of crown ethers, Lariat ethers, Podands, Cryptands, Spherands, Calixarenes, Cyclodextrins, Cyclophanes, Cryptophanes, Carcerands and hemicarcerands.

UNIT – V 12 hours
Supramolecules as transport and carrier design carrier: Transport processes and carrier design Carrier: Mediated transport, Cation transport processes–Cation carriers, Anion transport processes–anion carriers, Coupled processes, Molecular and supramolecular devices, Supramolecular ionic devices, Supramolecular photochemistry, Supramolecular electronic devices, Rational design, Molecular paneling, Supramolecular reactivity and catalysis.
Applications of supramolecular chemistry: Nanoscience applications, Metals in medicine: Metal deficiencies and diseases, Toxic effects of metals, Metals used for diagnosis and

chemotherapy with particular reference to anticancer drugs, Platinum complexes in cancer therapy: cis-platin and its mode of action.

REFERENCES

1. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, Panima Publishing Company, New Delhi, 1997.
2. W. Kaim and B. Schewederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley & Sons, New York, USA, 2013.
3. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry* 1st South Asia Ed., Viva books Pvt. Ltd, 2007.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry - Principles of Structure and Reactivity* 4th Ed., Pearson Education, 2006,.
5. P. Behrens and E. Bauerlein, *Hand Book of Biomineralization*, 1st Ed., Vol. 1 & 2, Wiley-VCH, 2007.
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7. J. M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, Wiley VCH, 1995.
8. P. D. Beer, P. A. Gale and D. K. Smith, *Supramolecular Chemistry*, Oxford University Press, 1999.
9. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, Wiley, 2000.
10. A. Bianchi, K. B. James and E. G. Espana, *Supramolecular Chemistry of Anions*, Wiley-VCH, 1997.
11. M. Fujita, *Molecular Self-assembly, Organic Versus Inorganic Approaches*, Springer, 2000.
12. J. P. Collman, L. S. Hegsdus, J. R. Norton and R. G. Finke, *Principles and Applications of Organotransition Metal Chemistry*, University Science Books.
13. P. Powell, *Principles of Organometallic Chemistry*, 2nd Ed., ELBS, 1991.
14. R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 6th Ed., Wiley, 2014.
15. A. J. Pearson, *Transition Metal-Stabilized Carbocations in Organic Synthesis*, Wiley, 2010.
16. M. Bochmann, *Organometallics and Catalysis: An Introduction*, OUP Oxford; UK Ed., 2014
17. R. C. Mehrotra, *Organometallic Chemistry: A Unified Approach*, 2nd Ed., New Age International, New Delhi, 2000.
18. B. D. Gupta and A. J. Elias, *Basic Organometallic Chemistry, Concepts, Syntheses and Applications*, University Press, 2010.
19. C. Elschenbroich and A. Salzer, *Organometallic Chemistry*, 2nd Ed., Weinheim, 1992.

Semester: IX
Course Name: Selected Topics in Physical and Inorganic Chemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**
Irreversible thermodynamics: Phenomenological laws and Onsager's reciprocity relations, Conservation of mass and energy in closed and open systems, Entropy production due to heat flow, Entropy production in chemical reactions, Entropy production and entropy flow in open systems, Principle of microscopic reversibility, Verification of Onsager's relations, Electrokinetic effects, Thermomolecular pressure difference and Thermomechanical effect, Application of irreversible thermodynamics to biological systems.

UNIT – II **12 hours**
Elementary numerical methods: Introduction to numerical methods, Taylor's theorem, Expansion of functions, Finding roots of an equation, Newton-Raphson method, Basic ideas of interpolation, Newton's forward and backward interpolation.
Computational chemistry-I: Concept of potential energy surface, Concept of methods and basis sets, Z-matrices, Equilibrium structure, Geometry optimization, Convergence criteria, Frequency calculation, Transition state calculations, Charge population analysis, Calculation of thermodynamic parameters.

UNIT – III **12 hours**
Basic computer programming: Programming language: Basic knowledge of Fortran 90: Data statements, logical and arithmetic expressions, Implicit and explicit data typing, Mix-mode arithmetic, Library functions, I-O statements, Implementation of loops, Nested loops, Control statements, Format specifications.

UNIT – IV **12 hours**
Inorganic clusters: Isolobal analogs of *p*-block and *d*-block clusters, Limitations and exceptions, Clusters having interstitial main group elements, Cubane clusters, Naked and zintl clusters, Molecular clusters in catalysis, Clusters to materials, Boron-carbides and Metal-borides,
Inorganic fibers: Introduction, Properties, Classification, Asbestos fibers, Optical fibers, Carbon fibers, Applications.

UNIT –V **12 hours**
Metal organic frameworks: Introduction to MOFs: Design, Synthesis, Structure and reactivity, Importance of Large-pore crystalline open frameworks, Post-synthetic modification of MOF, Functionalization and characterization: MOF Patterns, MOF immobilized thin films, Polymer MOF hybrid membranes (Crystals and Chains), Luminescent MOFs: Ligand-based luminescence in MOF, Metal based luminescence: LMCT, MLCT & MMCT in MOFs, Applications: Gas separation and storage (H_2, methane), CO_2 capture (from Flue gases, Natural gas and Syngas).

REFERENCES

1. I. Prigogine, *Introduction to Thermodynamics of irreversible Processes*, John Wiley, 3rd Ed., 1968.
2. I. N. Levine, *Quantum Chemistry*, Pearson, 7th Ed., 2013.
3. N. S. Ostlund and A. Szabo, *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*, Dover Publications, 1996.

4. Donald A. McQuarrie and John D. Simon, *Physical Chemistry: A Molecular Approach*, Viva Student Ed., 2011.
5. Donald A. McQuarrie, *Quantum Chemistry,* Viva Student Ed., 2014.
6. C. J. Cramer, *Essentials of Computational Chemistry-Theories and Models*, John Wiley and Sons Ltd., 2nd Ed., 2004.
7. F. Jensen, *Introduction to Computational Chemistry*, John Wiley and Sons Ltd., 3rd Ed., 2017.
8. D. C. Young, *Computational Chemistry-A Practical Guide for Applying Techniques to Real-World Problems*, John Wiley and Sons Ltd., 2001.
9. K. F. Purcell and J. C. Kotz, *Introduction to Inorganic Chemistry*, Holt-Saunders, Japan, 1982.
10. G. R. Chatwal, *Inorganic Polymers*, Himalaya Publisher, 2011.
11. J. E. Mark, H. R. Allcock and R. West, *Inorganic Polymers*, Prentice Hall, 1992.
12. N. H. Ray, *Inorganic Polymers*, London, New York, Academic Press, 1978.
13. D. M. P. Mingos and D. J. Wales, *Introduction to Cluster Chemistry*, Prentice Hall, 1990.
14. T. P. Fehlner, J. F. Halet and J. Y. Saillard, *Molecular Clusters: A Bridge to Solid-State Chemistry*, Cambridge University Press, 2007.
15. C. E. Housecroft, *Metal-Metal Bonded Carbonyl Dimers and Clusters*, Oxford Chemistry Primers (44), Oxford, University Press, 1996.
16. Kulkarni and K. Sulabha, *Nanotechnology: Principles and Practice*, Springer, 2015.

Semester: X
Course Name: Project/Dissertation
Course Code: **12 Credits (0-0-24)**

In continuation to the Project (Phase I), the students will complete their project work by solving their research problem. The research finding will be documented and a dissertation will be submitted. The students will deliver a power point presentation at the end of semester examination.

Semester: X
Course Name: Green Chemistry (Elective I)
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
Introduction to green chemistry: Definition, Principles of green chemistry, Ideal synthesis, E-factor, Atom economy, Atom economic (rearrangement and addition reactions) and uneconomic reactions (substitution and elimination reaction), Need, development and vision of green chemistry, Advantages over conventional methods, Modern variants in green synthesis, Step economy, Introduction to multicomponent reactions and Domino reactions.

UNIT – II 12 hours
Green synthesis/reactions: Comparative study of conventional and green protocols of Wittig, Bouveault, Heck, Michael addition, Darzen, Diels-Alder reaction, Thiamine mediated acyloin condensation, Baeyer-Villiger oxidation, Claisen rearrangement, Hantzsch synthesis, Ugi reaction, Click reactions, Combinatorial chemistry, Green synthesis of nanoparticles, Selected examples from US Presidential Green Chemistry Challenge Award Winners.

UNIT – III 12 hours
Reactions in unconventional medium: Pollution due to solvents, Global effect of solvent usage, Need for green solvents, Aqueous medium: Enhancement of selectivity, efficiency, and industrial applicability, Ionic liquids, Glycerol, Polyethylene glycol, Supercritical fluids, Solvent-free reactions, Fluorous phase reactions.

UNIT – IV 12 hours
Heterogeneous catalysis: Introduction to green catalysis, Heterogeneous catalysts, Advantages of solid catalysts or reagents, Use of zeolites, silica, alumina, clay, amberlyst, montmorillonite, polymers, cyclodextrin supported catalysts, Solid acids, Ion exchange resins, Advantages of solid acids over mineral acids, Supported metal oxides, Rare earth triflates, Physisorbed and Chemisorbed solid acid catalysis, Biocatalysts, Baker's yeast.

UNIT – V 12 hours
Nonconventional energy sources: Microwave assisted reactions, advantage of microwave exposure, specific effects of microwaves, selected microwave-assisted condensations reactions, oxidations, reductions reactions and multicomponent reactions, Ultrasound assisted reactions, Ball milling, Continuous flow reactor, Photochemical reactions.

REFERENCES

1. P. Tundo, A. Perosa and F. Zucchini, *Methods and Reagents for Green Chemistry*, Wiley, New Jersey, 2007.
2. M. Rai and C. Posten, *Green Biosynthesis of Nanoparticles Mechanisms and Application* CABI, 2013.
3. A. S. Matlack, *Introduction to Green Chemistry*, Marcel Dekker, Inc., New York, 2001.
4. A. Patti, *Green Approaches to Asymmetric Catalytic Synthesis*, Springer, 2011.
5. V. K. Ahluwalia, *Green Chemistry: Environmentally benign reaction*, Boca Raton, FL: CRC, Taylor & Francis, 2008.
6. P. T. Anastas and R. H. Crabtree, *Handbook of Green Chemistry, Green Catalysis, Homogeneous Catalysis*, Wiley, 2014.

Semester: X
Course Name: Computational Chemistry (Elective II)
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**
Programming in FORTRAN-I: Program design (algorithm), organization of program, data types and integer constants, complex constanta, logical constants, variables, implicit and explicit data typing, expressions and hierarchy of operations, mix-mode arithmatic, library functions, input/output specification.

UNIT – II **12 hours**
Programming in FORTRAN-II: Formatting, unconditional transfers, conditional statements and constructs, GO TO/ IF statements, relational operators, block if structure, else if construct, do loops, nesting, variables and arrays, parameter/data statements, common blocks, read/write by opening files, subroutines and construction of large program.

UNIT – III **12 hours**
Computational chemistry-II: Review of electronic structure theory: Hartree-Fock, MP2, Density Functional Theory, Configuration Interaction, Coupled-Cluster methods and Multi-Reference methods, Basis sets, Convergence, Geometry optimization, Balance between accuracy and computational time. Representative examples.

UNIT – IV **12 hours**
Computational chemistry-III: Computation of force constant, IR and RAMAN frequency calculations, Location of saddle point, intrinsic, Intrinsic reaction coordinates, Scanning the potential energy surfaces, Population analysis, NBO analysis, Calculation of thermodynamic parameters, Calculation of molecular excited electronic states. Representative examples.

UNIT – V **12 hours**
Numerical differentiation and integration: Taylor's theorem, Expansion of functions, Remainder, Mean value and Extreme value theorems, Discrete average value theorem. Numerical Differentiation (first and second derivatives), Numerical integration of a definite integral. Quadrature rule, Trapezoidal and Simpson’s one-third rule. Numerical solution of coupled differential equation using Runge Kutta method. LU factorization.

REFERENCES

1. C. J. Cramer, *Essentials of Computational Chemistry-Theories and Models*, John Wiley and Sons Ltd., 2nd Ed., 2004.
2. F. Jensen, *Introduction to Computational Chemistry*, John Wiley and Sons Ltd., 3rd Ed., 2017.
3. On-line manual of *Gaussian 16* and *GAMESS.* www.gaussian.com and www.msg.ameslab.gov/gamess
4. K. V. Raman, *Computers in Chemistry*, Tata McGraw Hill Education, 1st Ed., 2004.
5. V. Rajaraman, *Computer programming in FORTRAN*, Prentice Hall, 1994.
6. William H. Press, Saul A. Teukolsky , William T. Vetterling and Brian P. Flannery, *Numerical Recipes in Fortran 90: The Art of Scientific Computing*, Cambridge University Press, 2nd Ed., 1996.

Semester: X
Course Name: Organometallic Chemistry (Elective III)
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours

Structure and bonding in organometallic: Organometallic: Definition and classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicenter bonds), 16 and 18 electron rule and its limitations, Classification of organometallic compounds by bond type, Nomenclature, Metal-olefin complexes, Ziese's salt, EAN rule as applied to carbonyl, Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d-metal ions, Synergic effects (VB approach), MO diagram of CO can be referred for synergic effect to IR frequencies.

UNIT – II 12 hours

Chemistry of organometallic compounds: Synthesis and reactions of organomagnesium (Grignard reagent), Organomanganese, Organoaluminium, Organotin, Organozinc, Organolithium (*n*-BuLi, PhLi) reagents.

Cyclopentadienyl metal complexes: Metallocenes-Electronic structure and bonding in Ferrocene-Synthesis, Physical and spectroscopic properties of metallocenes.

Transition metal–*π* complexes

Transition metal–*π* complexes with unsaturated organic molecules like alkenes, Alkynes, Allyls, Diene and arene complexes, Preparation, Properties, Chemical reactions, Nature of bonding and structural properties.

UNIT – III 12 hours

Compounds of transition metal-carbon multiple bonds: Alkylidenes, Alkylidynes: Low valent (Fischer) and high valent (Schrock) carbenes and carbines: Synthesis, Nature of bond, Structural characteristics, Nucleophilic and electrophilic reactions of the ligands and applications.

Carbenes: N-heterocyclic carbenes, Fischer carbenes, Schrock carbenes, Carbynes, Isolobal analogy, Metal-metal bond, Transition metal clusters.

Unit IV: 12 hours

Reaction mechanism and catalysis: Homogeneous catalysis: Introduction, Properties of catalysis, Types of reactions in homogeneous catalysis (Oxidative addition, Reductive elimination, Insertion, Hydride elimination, Abstraction), Hydroformylation, Hydrogenation of olefins, Isomerisation of olefins, Oxo-process, Wacker process, Monsanto acetic acid synthesis, Monsanto *L*-Dopa synthesis, Water gas shift reaction, Carbonylation, Template synthesis, Alkene hydrosilation. Heterogeneous catalysis: Introduction, Fischer-Tropsch reaction, Ziegler-Natta catalysis.

Unit IV: 12 hours

Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2-olefin, η^3-allyl and dienyl complexes, Non-rigid molecules in different coordination geometry, Fluxional molecules, *σ*–bonded ligands.

Transition metal compounds with bonds to hydrogen: Chemistry of transition metal compounds with bonds to hydrogen: Types, synthesis and chemical reactions, Aluminohydrides and borohydrides, C-N bond coupling reactions and asymmetric hydrogenations.

Biological applications and environmental aspects of organometallic compounds: Introduction, Organometallics in medicine, Agriculture, Horticulture and environmental aspects.
Applications of organometallics in organic synthesis: C-C coupling reactions (Heck, Sonogoshira, Suzuki etc).

REFERENCES

1. J. P. Collman, L. S. Hegsdus, J. R. Norton and R. G. Finke, *Principles and Applications of Organotransition Metal Chemistry*, University Science Books.
2. P. Powell, *Principles of Organometallic Chemistry*, 2nd Ed., ELBS, 1991.
3. R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 6th Ed., Wiley, 2014.
4. A. J. Pearson, *Transition Metal-Stabilized Carbocations in Organic Synthesis*, Wiley, 2010.
5. M. Bochmann, *Organometallics and Catalysis: An Introduction*, OUP Oxford; UK Ed., 2014
6. R. C. Mehrotra, *Organometallic Chemistry: A Unified Approach*, 2nd Ed., New Age International, New Delhi, 2000.
7. B. D. Gupta and A. J. Elias, *Basic Organometallic Chemistry, Concepts, Syntheses and Applications*, Basic.Pubs: University Press, 2010.
8. C. Elschenbroich and A. Salzer, *Organometallic Chemistry*, 2nd Ed., Weinheim, 1992.
9. B. C. Chapman all, *Heterogeneous Catalysis*, 2nd Ed., 1987.
10. G. W. Parshall and S. D. Ittel, Homogenous Catalysis: the Applications and Chemistry of Catalysis by Soluble Transition Metal Complexes, 2nd Ed., Wiley, 1992.
11. J. P. Collman, L. S. Hegsdus, J. R. Norton and R. G. Finke, *Principles and Applications of Organotransitiion Metal Chemistry*, University Science Books.
12. C. M. Lukehart, *Fundamental Transition Metal Organometallic Chemistry*, Brooks/Cole Pub Co, 1985.
13. J. M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, Wiley VCH, 1995.
14. R. M. Roat-Malone, *Bioinorganic Chemistry: A Short Course*, John Wiley & Sons, 2007.
15. P. D. Beer, P. A. Gale and D. K. Smith, *Supramolecular Chemistry*, Oxford University Press, 1999.
16. J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, Wiley, 2000.
17. A. Bianchi, K. B. James and E. G. Espana, *Supramolecular Chemistry of Anions*, Wiley-VCH, 1997.
18. M. Fujita, *Molecular Self-assembly, Organic Versus Inorganic Approaches*, Springer, 2000.

Semester: X
Course Name: Solid State Chemistry (Elective IV)
Course Code: 4 Credits (3-1-0)

UNIT – I 12 hours
General principles of solid state reactions: Solid state reactions and Crystal defects- Perfect and imperfect crystals, Intrinsic and extrinsic defects, Point defects (Schottky and Frenkel defects), Thermodynamics of Schottky and Frenkel defect formation, Colour centres, Line defects: Edge dislocation and Screw dislocation, Plane defects: Grain boundary and Staking faults, Non-stoichiometry and defects. Topochemical control of solid state organic reactions, New superconductors.
Solid solutions: Substitutional solid solutions, interstitial solid solutions, more complex solid solutions mechanisms, requirements for solid solutions and formation.

UNIT – II 12 hours
Preparative methods and crystal symmetry: Preparation of materials in solid state: Precursor, ceramic, sol-gel, hydrothermal, electrochemical reduction methods, vapour phase transport and high pressure methods, preparation of thin films, growth of single crystals, Closed packed structures: cubic close packing and hexagonal close packing, Some important structure types : NaCl, ZnS, CsCl and perovskite ($SrTiO_3$).

UNIT – III 12 hours
Structure of solids: Crystal systems, Bravais lattice, Lattice planes, Miller indices and directions, Symmetry: Point symmetry, space symmetry and point groups, Representation of point groups and examples (orthorhombic point groups: 222, mm2, mmm), Space groups.

UNIT – IV 12 hours
Electronic and ionic conduction: Metals, Insulators and Semiconductors, Electronic structure of solids, Chemical and physical approaches-Band theory, Band structure of metals, Insulators and semiconductors, Intrinsic and extrinsic semiconductors, Doping of semiconductors, P N junction, Band structure in organic solids, Colour in organic solids, Ionic conductivity in solids, Solid electrolytes, Fast ion conductors (α-AgI, β-Alumina, Stabilized zirconia).

UNIT – V 12 hours
Magnetic Properties: Classification of materials, Behaviour of substances in a magnetic field, Effect of temperature: Curie and Curie-Weiss laws, Calculation of magnetic moments, Mechanisms of ferro and anti-ferromagnetic ordering, Super exchange and double exchange, Theory of diamagnetism, Langevin's theory of paramagnetism, Quantum mechanical approach for paramagnetism, Theory of ferromagnetism, Antiferro and ferri magnetism, Ferromagnetic domains and hysteresis, Soft and hard magnetic materials.

REFERENCES

1. A. R. West, *Solid State Chemistry*, Wiley Student Ed., (Indian Ed.). 2003.
2. I. N. Levin, *Physical Chemistry*, 6^{th} Ed. Mc Graw Hill Education, 2011.
3. C. N. R. Rao and J. Gopalakrishnan, *New Directions in Solid State Chemistry*, 2^{nd} Ed., Cambridge University Press. 1987.
4. R. L. Catin, *Magnetochemistry*, Springerverlag, Berlin.
5. N. B. Hannay, *Solid State Chemistry*, Prentice Hall (India) Ltd., New Delhi, 1967.

Semester: X
Course Name: Nano Chemistry
Course Code: **4 Credits (3-1-0)**

UNIT – I **12 hours**

Introduction to nanomaterials: History of nanoscience, Definition of Nanometer, Nanomaterials and Nanotechnology, Classification of nanomaterials, Metal clusters, Metal nanoparticles, Semiconductor nanoparticles, Polymer nanostructures, Size effects on surface area, Surface energy, Optical, Electrical, Mechanical and Catalytic properties, Quantum confinement effect, Quantum dots, Nanowires, Nanorods and Nano film, Stabilizing agents, Types and its interaction with nanoparticles, Zeta potential.

UNIT – II **12 hours**

Synthesis of nanomaterials: Physical methods: Physical vapour deposition, Laser ablation, Laser pyrolysis, Sputter deposition: DC, RF and Magnetron sputtering, Chemical vapour deposition, Chemical Methods: Colloidal in solution, Nucleation and growth of nanoparticles, Synthesis of metal and semiconductor nanoparticles via colloidal route, Sol-gel method, Hydrothermal method, Microemulsion method, Sonochemical method and microwave method, Biogenic Methods, Synthesis using microorganism and plant extracts.
Self-assembly of nanomaterials: Mechanism of self assembly, Self assembly of nanoparticles using organic molecules, Self assembly in biological systems and Inorganic materials.

UNIT – III **12 hours**

Carbon nanomaterials: Fullerenes synthesis and properties, Carbon nanotubes (CNT), Types of CNT, Synthesis and growth mechanism, Graphene synthesis and properties, Porous materials, Porous silicon: Synthesis, mechanism and properties, Mesoporous silica: Synthesis and properties, Mesoporous carbon nanomaterials: Synthesis, properties and applications.
Core-shell semiconducting nanoparticles: Different types of core-shell, Synthesis, Surface functionalization of core-shell, Properties.
Aerogels and hydrogels: Types, fabrication methods and properties.

UNIT – IV **12 hours**

Characterization of nanomaterials: Diffraction Techniques: X-ray diffraction, Dynamic light scattering, Spectroscopic techniques: Absorption, fluorescence, Infrared, Raman and X-ray photoelectron spectroscopy, Microscopic techniques: Scanning probe, Scanning and Transmission electron microscope.
Applications of nanomaterials: Dye sensitized solar cell, Polymer solar cell, Fuel cell, Optical (colorimetric and fluorescence) sensor, Electrochemical sensor, Water purification.

UNIT – V **12 hours**

Nanotechnology in food, medicine and health sciences: Nano particle based drug delivery systems, Ultra sound triggered Nano/Microbubbles, Regenerative medicine, Nanoimmuno conjugates, Biosensors, Optical biosensors based on nanoplasmonics, Nanobiosesors, Cyclodextrin based nanomaterials, Bioavailability and delivery of nutraceuticals and functional foods using nanotechnology, Polymer-based nanocomposites for food packaging, Toxicity and environmental risks of nanomaterials.

REFERENCES

1. C. N. R. Rao, A. Muller and A. K. Cheetham, Eds., *The Chemistry of Nanomaterials*, Wiley-VCH, Germany, 2004.
2. G. Ozin, A. Arsenaut, Eds., *Nanochemistry: A Chemical Approach to Nanomaterials*, Royal Society of Chemistry, London, 2005.
3. T. Pradeep, *Nano: The Essentials, Understanding Nanoscience and Nanotechnology*, McGraw Hill Education, New Delhi, 2007.
4. M. S. Ramachandra Rao and Shubra Singh, *Nanoscience and Nanotechnology: Fundamentals to Frontiers*, Wiley, 2014.
5. S. K. Kulkarni, *Nanotechnology: Principles and Practices,* Springer, 2011.

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