VIMALA COLLEGE (AUTONOMOUS), THRISSUR

(Affiliated to University of Calicut)

M.Sc. DEGREE PROGRAMME IN CHEMISTRY

UNDER CHOICE BASED CREDIT AND SEMESTER SYSTEM

SCHEME AND SYLLABI

2016 ADMISSION ONWARDS

CORE COURSES & ELECTIVE COURSES

VIMALA COLLEGE (AUTONOMOUS)

M.Sc. CHEMISTRY

Pattern of the Programme

a) The name of the programme shall be M.Sc. Chemistry.

b) The programme shall be offered in four semesters within a period of two academic years.

c) Details of the programme offered for the programme are given in Table 1. The programme shall be conducted in accordance with the programme pattern, scheme of examination and syllabus prescribed. Of the 25 hours per week, 12 hours shall be allotted for theory, 12 hours for practical and 1 hour for seminar.

Course structure

Theory Courses

In the first three semesters there will be four theory courses and in the fourth semester three theory courses. All the theory courses in the first and second semesters are core courses. In the third semester there will be three core theory courses and one elective theorycourse. In the fourth semester there will be two core theory courses and one elective theory course..However a student may be permitted to choose any other elective course in the third and fourth semesters, without having any lecture classes. All the theory courses inthe first, second and third semesters are of 3 credits while the theory courses in the fourth semester are of 4 credits

Practical Courses

In each semester, there will be three core practical courses. However the practicalexaminations will be conducted only at the end of second and fourth semesters. At the end of second semester, three practical examinations with the codes VPCH1PO1 & VPCH2PO4, VPCH1PO2 & VPCH2PO5 and VPCH1PO3 & VPCH2PO6 will be conducted. Practical examinations for the codes VPCH3PO7 & VPCH4P10, VPCH3PO8 & VPCH4P11 and VPCH3PO9 & VPCH4P12 will be conducted at the end of fourth semester. Each practical examination will be of six hour duration and 4 credits.Three hours per week in the fourth semester are allotted for conducting individual project work by the students under guidance of a faculty and it can be treated as practical hours while working out the workload of teachers.

Project and Viva Voce

Each student has to perform an independent research project work during the programme under the guidance of a faculty member of the college/ scientists or faculties of recognised research institutions. Projects done in the quality control or quality analysis division of the industries will not be considered. At the same time, projects done in the R & D division of reputed industry can be considered. Each student has to submit three copies of the project dissertation for valuation at the end of fourth semester. After the valuation one copy may be returned to the student, one may be given to the project supervisor and the third one should be kept in the department/college library. Evaluation of the project work (4 credits) will be done on a separate day at the end of fourth semester, after the theory examinations. Viva voce on the project will also be done on the same day.Viva voce examinations, based on the theory and practical courses, will be conducted at the end of second and fourth semesters (2credits each), on a separate day.

Credit distribution in each semester

TABLE I

Semester	Course Code	Course Title	Instruction/ week	Credits
I	VPCH1C01	Basic concepts in quantum chemistry & group theory	3	3
	VPCH1C02	Elementary inorganic chemistry	3	3
	VPCH1C03	Structure and reactivity of organic compounds	3	3
	VPCH1C04	Thermodynamics, kinetics and catalysis	3	3
	VPCH1PO1	Inorganic chemistry Practical I	4	-
	VPCH1PO2	Organic chemistry practical I	4	-
	VPCH1PO3	Physical chemistry practical I	4	-
		Total credits	**Core**	**12**
II	VPCH2CO5	Applications of quantum mechanics & group theory	3	3
	VPCH2CO6	Coordination chemistry	3	3
	VPCH2CO7	Organic reaction mechanisms	3	3
	VPCH2CO8	Electrochemistry, Solid state chemistry & Statistical thermodynamics	3	3
	VPCH2PO4	Inorganic chemistry practical II	4	4
	VPCH2PO5	Organic chemistry practical II	4	4
	VPCH2PO6	Physical chemistry practical II	4	4
	VPCH2VO1	Viva voce		2
		Total credits	**Core** **Viva**	**24** **2**
III	VPCH3CO9	Molecular spectroscopy	3	3
	VPCH3C10	Organometallic & Bioinorganic chemistry	3	3
	VPCH3C11	Organic transformations & reagents	3	3
	VPCH3PO7	Inorganic chemistry practicals III	4	
	VPCH3PO8	Organic chemistry practicals III	4	
	VPCH3PO9	Physical chemistry practicals III	4	
	VPCH3EO1	Synthetic organic chemistry (Elective)	3	3
		Total credits	**Core** **Elective**	**9** **3**

IV	VPCH4C12	Advanced topics in chemistry	4	4
	VPCH4C13	Instumental methods of analysis	4	4
	VPCH4P10	Inorganic chemistry practical IV	3	4
	VPCH4P11	Organic chemistry practical IV	3	4
	VPCH4P12	Physical chemistry practical IV	3	4
	VPCH4E05	Industrial Catalysis (Elective)	4	4
	VPCH4Pr01	Research Project	3	4
	VPCH4V02	Viva Voce		2
		Total Credits	**Core** **Elective** **Project** **Viva**	**20** **4** **4** **2**
TOTAL CREDITS OF THE PROGRAMME			**CORE** **ELECTIVE** **PROJECT** **VIVA VICE** ***TOTAL CREDITS***	**65** **7** **4** **4** **80**

Semester : I

Course Code : VPCH1CO1

Course Title : QUANTUM CHEMISTRY AND GROUP THEORY

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH1CO1 - QUANTUM CHEMISTRY AND GROUP THEORY (3Credits, 54 hrs)

Unit 1: Introduction to Quantum Mechanics (9hrs)

Failure of classical mechanics: Black body radiation and Planck's quantum postulate. Einstein's photoelectric equation, Compton effect, Zeeman effect- the need for quantum mechanics. Uncertainty principle, Schrodinger's wave mechanics, Deduction of Schrodinger wave equation from classical wave equation- Detailed discussion of postulates of quantum mechanics – State function or wave function postulate, Born interpretation of the wave function, well behaved functions, orthonormality of wave functions; Operator postulate, operator algebra, linear and nonlinear operators, Laplacian operator, Hermitian operators and their properties, eigen functions and eigen values of an operator; Eigen value postulate, eigen value equation, eigen functions of commuting operators; Expectation value postulate; Postulate of time-dependent Schrödinger equation of motion, conservative systems and time-independent Schrödinger equation. Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta ((Lx, Ly, Lz), commutation relations between these operators, Ladder operator method for angular momentum, space quantization.

Unit 2: Quantum Mechanics of Translational & Vibrational Motions (9hrs)

Free particle in one-dimension; Particle in a one-dimensional box with infinite potential walls, important features of the problem; Particle in a one-dimensional box with one finite potential wall, Particle in a rectangular well, (no derivation), Significance of the problem, Introduction to tunneling; Particle in a three dimensional box, Separation of variables, degeneracy,Bohr's correspondence principle. One-dimensional harmonic oscillator (complete treatment):- Method of power series, Hermite equation and Hermite polynomials, recursion relation, wave functions and energies, important features of the problem, harmonic oscillator model and molecular vibrations

Unit: 3 Quantum Mechanics of Rotational Motion (9hrs)

Co-ordinate systems: - Cartesian, cylindrical polar and spherical polar coordinates and their relationships. Planar rigid rotor (or particle on a ring), the Phi-equation, solution of the Phi-equation, One particle Rigid rotator (non planar rigid rotator or particle on a sphere) (complete treatment): Angular momentum in spherical polar co-ordinate, The wave equation in spherical polar coordinates, wave functions in the real form; separation of variables, the Phi-equation and the Theta-equation and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials, Rodrigue's formula, spherical harmonics (imaginary and real forms),Converting imaginary functions to real form, polar diagrams of spherical harmonics. Spherical harmonics as eigen functions of angular momentum operators Lz, L^2

Unit 4: Quantum Mechanics of Hydrogen-like Atoms (9hrs)

Potential energy of hydrogen-like systems, the wave equation in spherical polar coordinates, separation of variables, the R, Theta and Phi equations and their solutions, Laguerre and associated Laguerre polynomials, wave functions and energies of hydrogen-like atoms, orbitals, radial functions and radial distribution functions and their plots, angular functions (spherical harmonics) and their plots. The postulate of spin by Uhlenbeck and Goudsmith, Dirac's relativistic equation for hydrogen atom and discovery of spin (qualitative treatment), spin orbitals, construction of spin orbitals from orbitals and spin functions.

Unit 5: Foundations of Group Theory & Molecular Symmetry (9hrs)

Basic principles of group theory - the defining properties of mathematical groups, finite and infinite groups, Abelian and cyclic groups, group multiplication tables (GMT), similarity transformation, sub groups & classes in a group.

Molecular Symmetry & point groups - symmetry elements and symmetry operations in molecules, relations between symmetry operations, complete set of symmetry operations of a molecule, point groups and their systematic identification, GMT and classes of point groups;

Mathematical preliminaries - matrix algebra, addition and multiplication of matrices, inverse of a matrix, square matrix, character of a square matrix, diagonal matrix, direct product and direct sum of square matrices, block factored matrices, solving linear equations by the method of matrices;

Matrix representation of symmetry operations.

UNIT 6: Representations of Point Groups & Corresponding Theorems (9hrs)

Representations of point groups - basis for a representation, representations using vectors, atomic orbitals and Cartesian coordinates positioned on the atoms of molecule (H_2O as example) as bases, reducible representations and irreducible representations (IR) of point groups, construction of IR by reduction (qualitative demonstration only), Great Orthogonality Theorem (GOT) (no derivation) and its consequences, derivation of characters of IR using GOT, construction of character tables of point groups (C_{2V}, C_{3V}, C_{2h} and C_{4V} and C_3 as examples), nomenclature of IR - Mulliken symbols, symmetry species;
Reduction formula - derivation of reduction formula using GOT, reduction of reducible representations, (e.g., $_{cart}$) using the reduction formula;
Relation between group theory and quantum mechanics – wavefunctions (orbitals) as bases for IR of point groups.

Reference for Units 1 to 4

1. F.L. Pilar, *Elementary Quantum Chemistry* , McGraw-Hill, 1968.
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.,
3. I.N. Levine, *Student Solutions Manual for Quantum Chemistry 6th Edition*, Pearson Education Inc., 2009.
4. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics* , 4th Edition, Oxford University Press, 2005.
5. M.W. Hanna, *Quantum Mechanics in Chemistry*, 2nd Edition, W.A. Benjamin Inc., 1969.
6. Donald, A. McQuarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition,Viva books, 2003).
7. Thomas Engel, Quantum Chemistry & Spectroscopy, Pearson Education, 2006.
8. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.
9. Horia Metiu, *Physical Chemistry – Quantum Mechanics*, Taylor & Francis, 2006.
10. A.K. Chandra, *Introduction to Quantum Chemistry* , 4th Edition, Tata McGraw-Hill, 1994.
11. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, 1935 (A good source book for many derivations).
12. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.
13. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.
14. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.
15. C.n. datta, *lectures on chemical bonding and quantum chemistry*, prism books pvt. Ltd., 1998.
16. Jack simons, *an introduction to theoretical chemistry*, cambridge university press, 2003.

For units 5&6

1. F.a. cotton, *chemical applications of group theory*, 3rd edition, john wiley &sons Inc., 2003.
2. H. H. Jaffe and m. Orchin, *symmetry in chemistry*, john wiley &sons inc., 1965.
3. L.h. hall, *group theory and symmetry in chemistry*, mcgraw hill, 1969.
4. R. Mcweeny, *symmetry: an introduction to group theory and its applications*, Pergamon press, london, 1963.
5. P.h. walton, *beginning group theory for chemistry*, oxford university press inc., new York, 1998.
6. Mark ladd, *symmetry & group theory in chemistry*, horwood 1998.
7. A. Salahuddin kunju & g. Krishnan, *group theory & its applications in chemistry*, phi Learning pvt. Ltd. 2010.
8. Arthur m lesk, *introduction to symmetry & group theory for chemists*, kluwer Academic publishers,2004.
9. K.veera reddy, *symmetry & spectroscopy of Molecules 2nd edn.*, new age international 2009.
10.a.w. joshi, *elements of group theory for physicists*, new age international publishers, 1997.

COURSE: QUANTUM MECHANICS AND GROUP THEORY

Credits: 3

Instructors: Susan Samuel,Anjali T R **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	STUDY THE POSTULATES OF QUANTUM MECHANICS	PSO I	U	P	8	0	0
2	Acquire knowledge about THE SYSTEMS 1-D BOX, 3-D BOX AND SIMPLE HARMONIC OSCILLATOR	PSO I	U	C	8	0	0
3	GENERATE IDEA ABOUT PARTICLE ON A RING AND SPHERE	PSO I	E	F	8	0	0
4	EVALUATE THE EIGEN FUNCTION AND EIGEN VALUE OF HYDROGEN LIKE ATOMS	PSO I	An	P	8	0	0
5	EXPLAIN THE SIMILARITY TRANSFORMATION	PSO I	An	P	3	0	0
6	DESCRIBE THE MOLECULAR SYMMETRY	PSO II	Ap	C	5	0	0
7	ELABORATE THE GREAT ORTHOGONALITYTHEOREM	PSO I	U	P	4	0	0
8	CONSTRUCTION OF CHARACTER TABLES OF POINT GROUPS	PSO II	Ap	F	4	0	0

Total hours of instruction 54

**Course Code : ** VPCH1CO2

Course Title : - ELEMENTARY INORGANIC CHEMISTRY (3 Credits, 54hrs)

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :
VPCH1CO2 - ELEMENTARY INORGANIC CHEMISTRY (3 Credits, 54hrs)

Unit 1: Molecular Structure and Bonding (9hrs)
Molecular topologies-shared and lone pair and Lewis structure..Resonance – Formal charge–hypervalence-electroneutrality principle-Isoelectronic molecules. Isolobal relationship. VSEPR theory, dπ–pπ bonds. Bent rule and energetics of hybridization. Bonding in metals, packing of atoms in metals, band theory of metals and metallic properties, insulators and semiconductors

Unit 2: Concepts of Acids and Bases (9hrs)
Major acid-base concepts, Arrhenius, Bronsted-Lowry, Solvent system, Lux-Flood, Lewis and Usanovich concepts. Classification of acids and bases as hard and soft. HSAB principle.-Theoretical basis of hardness and softness. Levelling effect, The Drago-Wayland equation, E and C parameters- Symbiosis. Applications of HSAB concept.

Chemistry of nonaqueous solvents- NH_3, SO_2, H_2SO_4, BrF_3, HF, N_2O_4 and HSO_3 F. Nonaqueous solvents and acid-base strength. Super acids –surface acidity.

Unit 3: Chemistry of Main Group Elements-I (9hrs)
Chemical periodicity-First and Second raw anomalies-The diagonal relationship-Periodic anomalies of the nonmetals and post-transition metals.

Allotropes of C, S, P. As, Sb, Bi, O and Se. Electron deficient compounds-Boron hydrides-preparation, reactions, structure and bonding. Styx numbers-closo, nido, arachno polyhedral structures. Boron cluster compounds-Wade's rule. Polyhedral borane anion-carboranes, metallaboranes and metallacarboranes. Borazines and borides.

Unit 4: Chemistry of Main Group Elements-II(9hrs)
Silicates and alumino silicates-Structure, molecular sieves-Zeolite. Silicones-Synthesis, structure and uses. Carbides and silicides. Synthesis, structure, bonding and uses of Phosphorous-Nitrogen, Phosphorous -Sulphur and Sulphur-Nitrogen compounds.

Unit 5: Chemistry of Transition and Inner Transition Elements (9hrs)
Heteropoly and isopoly anions of W, Mo, V.
Standard reduction potentials and their diagrammatic representations Ellingham diagram. Latimer and Frost diagrams. Pourbaix diagram.
Differences between 4f and 5f orbitals. Magnetic and spectroscopic properties. Uranyl compounds. Trans-actinide elements. Super heavy elements –production and chemistry.

Unit 6: Nuclear and Radiation Chemistry (9hrs)

Structure of nucleus: shell, liquid drop, Fermi gas, collective and optical models. Nuclear reaction: Bethe`s notation of nuclear process- Types-reaction cross section-photonuclear and thermonuclear reactions.

Nuclear fission: Theory of fission- neutron capture cross section and critical size. Nuclear fusion. Neutron activation analysis

Radiation chemistry: Interaction of radiation with matter. Detection and measurement of radiation- GM and scintillation counters – radiolysis of water- radiation hazards-radiation dosimetry.

References

1. N.N. Greenwood and A.Earnshaw, *Chemistry of Elements, 2/e, Elsevier* Butterworth-Heinemann,2005.

2. J.E.Huheey, E.A.Keiter, R.L.Keiter. O.K.Medhi. *Inorganic Chemistry, principles of Structure and reactivity*, Pearson Education, 2006.

3. G.L.Miessler, D.A.Tarr, *Inorganic Chemistry*, Pearson, 2010.

4. D.F.Shriver, P.W.Atkins, *Inorganic Chemistry*, Oxford University Press, 2002

5.William W Porterfield, *Inorganic Chemistry-A unified approach,* Academic Press,2005.

6. Keith F Purcell, John C Kotz, *Inorganic Chemistry*, Cengage Learning, 2010.

7. James E House, *Inorganic Chemistry,* Academic Press, 2008.

8. H.J.Arnikar, *Essentials of Nuclear chemistry*, New Age International, 2005.

9. Friedlander and J.W.Kennedy, *Introduction to Radiochemistry*, John Wiley and Sons, 1981.

10.S.Glastone, *Source Book on Atomic Energy, 3rd*edn., Affiliated East-West Press Pvt.Ltd., 1967.

COURSE CODE : VPCH1CO2

COURSE: ELEMENTARY INORGANIC CHEMISTRY (3 Credits, 54hrs)

Credits: 3

Instructors: Susan Samuel, Jidha K S **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Analyse molecular structures based on electroneutrality principle and VSEPR theory	PSO I	An	C	6	0	0
2	Study bonding involved in metals and their metallic properties	PSO I	U	F	6	0	0
3	Acquire knowledge about major acid-base concepts	PSO III	U	C	6	0	0
4	Evaluate electron deficient Boron compounds based on Wade's rule	PSO I	E	C	6	0	0
5	Understand about structure, bonding and synthesis of P-N,P-S,S-N compounds	PSO II	U	C	8	0	0
6	Draw the Ellingham, Latimer,Frost and Poubaix diagrams	PSO I	An	P	8	0	0
7	State the various theories to explain the structure of nucleus	PSO I	U	C	6	0	0
8	Describe the interaction of radiation with matter	PSO II	U	F	8	0	0

Total hours of instruction 54

**Course Code : **VPCH1CO3

Course Title : - STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS (3Credits, 54hrs)

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH1CO3 -STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS (3Credits, 54hrs)

Unit 1: Structure and Bonding in Organic Molecules (9hrs)

Nature of Bonding in Organic Molecules: Localized and delocalized chemical bonding, bonding weaker than covalent bond, cross- conjugation, resonance, rules of resonance, resonance hybrid and resonance energy, tautomerism, hyperconjugation, π-π interactions, pπ-dπ bonding (ylides).

Hydrogen bonding: Inter and intra-molecular hydrogen bonding. Range of the energy of hydrogen bonding. Effect of hydrogen bond on conformation, physical and chemical properties of organic compounds- volatility, acidity, basicity and stability. Stabilization of hydrates of glyoxal and chloral, and ninhydrin. High acid strength of maleic acid compared to fumaric acid. Electron donor-acceptor complexes, crown ether complexes, cryptates, inclusion compounds and cyclodextrins.

Hückel MO method. MO's of simple molecules, ethylene, allyl radical and 1,3-butadiene. Hückel rule and modern theory of aromaticity, criteria for aromaticity and antiaromaticity, MO description of aromaticity and antiaromaticity. Homoaromaticity. Aromaticity of annulenes and heteroannulenes, fused ring systems, fulvenes, fulvalenes, azulenes, pentalenes and heptalenes. Preparation of aromatic and antiaromatic compounds by different methods, stability of benzylic cations and radicals. Effect of delocalized electrons on pKa.

Unit 2: Structure and Reactivity (9hrs)

Transition state theory, Potential energy vs reaction co-ordinate curve, substituent effects (inductive, mesomeric, inductomeric, electomeric and field effects) on reactivity. Qualitative study of substitution effects in S_N1-S_N2 reactions. Neighbouring group participation, participation of carboxylate ion, halogen, hydroxyl group, acetoxy group, phenyl group and pi - bond. Classical and nonclassical carbocations

Basic concepts in the study of organic reaction mechanisms: Application of experimental criteria to mechanistic studies, kinetic versus thermodynamic control- Hammond postulate, Bell-Evans-Polanyi principle, Marcus equation, Curtin-Hammet principles, Acidity constant, Hammet acidity function.

Isotope effect (labeling experiments), stereochemical correlations. Semiquantitative study of substituent effects on the acidity of carboxylic acids. Quantitative correlation of substituent effects on reactivity. Linear free energy relationships. Hammet and Taft equation for polar effects and Taft's steric substituent constant for steric effect. Solvent effects.

Unit 3: Conformational Analysis – I (9hrs)

Factors affecting the conformational stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Conformation of acyclic compounds – Ethane, n-butane, alkene dihalides, glycols, chlorohydrines, tartaric acid, erythro and threo isomer.
cyclohexane–methyl and t-butyl cyclohexanes–flexible and rigid systems. Conformation of substituted cyclohexanone, 2-bromocyclohexanone, dibromocyclo hexanone, (cis & trans), 2-bromo-4,4-dimethyl cyclohexanone. Anchoring group and conformationaly biased molecules. Conformations of 1,4 -cis and -trans disubstituted cyclohexanes in which one of the substituent is 1-butyl and their importance in assessing the reactivity of an axial or equatorial substituent.

Unit 4: Conformational Analysis – II (9 hrs)
Effect of conformation on the course and rate of reactions in (a) debromination of dl and meso 2,3-dibromobutane or stilbene dibromide using KI. (b) semipinacolic deamination of erythro and threo 1,2-diphenyl-1-(p-chlorophenyl)-2-amino ethanol. (c) dehydro halogination of stilbene dihalide (dl and meso) and erythreo threo- bromo-1,2-diphenyl propane.

Effect of conformation on the course and rate of reactions in cyclohexane systems illustrated by: (a) S_N2 and S_N1 reactions for (i) an axial substituent, and (ii) an equatorial substituent in flexible and rigid systems. (b) E1, E2 eliminations illustrated by the following compounds. (i) 4-t-Butylcyclohexyl tosylate (cis and trans) (ii) 2-Phenylcyclohexanol (cis and trans) (iii) Menthyl and neomenthyl chlorides and benzene hexachlorides. (c) Pyrolytic elimination of esters (cis elimination) (d) Esterification of axial as well as equatorial hydroxyl and hydrolysis of their esters in rigid and flexible systems. (Compare the rate of esterification of methanol, isomenthol, neomenthol and neoisomenthol). (f) Esterification of axial as well as equatorial carboxyl groups and hydrolysis of their esters. (g) Hydrolysis of axial and equatorial tosylates. (h) Oxidation of axial and equatorial hydroxyl group to ketones by chromic acid.

Bredt's rule. Stereochemistry of fused, bridged and caged ring systems-decalins, norbornane, barrelene and adamantanes.

Unit 5: Stereochemistry (9hrs)
Conformation and configuration, Fischer, Newman and Sawhorse projection formulae and their interconversion. Concept of chirality, recognition of symmetry elements and chiral structures, conditions for optical activity, optical purity. Specific rotation and its variation in sign and magnitude under different conditions, relative and absolute configurations, Fisher projection formula, sequence rule – *R and S* notation in cyclic and acyclic compounds, Cahn-Ingold-Prelog (CIP) rule. Mixtures of stereoisomers; enantiomeric excess and diastereomeric excess and their determination. Methods of resolution diastereomers. Resolution of racemates after conversion into diastereomers; use of S-brucine, kinetic resolution of enantiomers, chiral chromatography.

Optical isomerism of compounds containing one or more asymmetric carbon atoms, enantiotopic, homotopic, diastereotopic hydrogen atoms, prochiral centre. Pro-R, Pro-S, Re and Si.

Optical isomerism in biphenyls, allenes and nitrogen and sulphur compounds, conditions for optical activity, R and S notations. Optical activity in cis-trans conformational isomers of 1,2-, 1,3- and 1,4-dimethylcyclohexanes .

Restricted rotation in biphenyls – Molecular overcrowding.
Chirality due to folding of helical structures.

Geometrical isomerism – E and Z notation of compounds with one and more double bonds in acyclic systems. Configuration of cyclic compounds-monocyclic, fused and bridged ring systems, inter conversion of geometrical isomers. Methods of determination of the configuration of geometrical isomers in acyclic acid cyclic systems, stereochemistry of aldoximes and ketoximes

Unit 6: Asymmetric Synthesis (9 hrs)
The chiral pool: alpha aminoacids in the synthesis of benzodiazepines, carbohydrates,(benzyl D mannose to-Swainsonine /preparation of Tomolol from D –Mannitol),Felkin –Ahn model and Cram's chelation control
Chiral auxiliaries : Oxazolidinones ,chiral sulphoxides in controlling the reduction of ketones , Camphor derivative in Diels Alder reaction and radical reactions
Chiral reagents: BINOL,Tartarates,Litihum di(1-phenylethyl)amide.
Chiral catalyst-Rhodium and Ruthenium catalyst with chiral phosphenes ligands like(R) BINAP,(R,R)DIOP.Enzymatic methods

References:

1. R. R. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A*, Springer, 5/e,2007.

2. M. B. Smith, J. March, *March's Advanced Organic Chemistry*, John Wiley & Sons, 6/e,2007.

3. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley, 1998.

4. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, 2/e, Oxford University Press,2012.

5. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2005.

6. M. S. Singh, *Advanced Organic Chemistry: Reactions and Mechanisms*, Pearson, 2013.

7. P. Sykes, *A Guide book to Mechanism in Organic Chemistry*, 6/e, Pearson, 2006.

8. C. K. Ingold, Structure and Mechanism in Organic chemistry, 2/e, CBS Publishers, 1994.

9. E. L. Eliel, S. H. Wilen and L. N. Mander, *Stereochemistry of Carbon Compounds*, John Wiley, 1997.

10. G. L. D. Krupadanam, *Fundamentals of Asymmetric Synthesis*, Universities Press, 2013.

11. Okuyama and Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press, 2013

12. S. Warren and P. Wyatt, *Organic Synthesis: The Disconnection Approach*, 2/e, John Wiley & Sons, 2008

COURSE CODE : VPCH1CO3

COURSE: STRUCTURE AND REACTIVITY OF ORGANIC COMPOUNDS (3 Credits, 54hrs)

Credits: 3

Instructors: Susan Samuel, Jidha K S **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Understand about hydrogen bonding and its effect on organic compounds	PSO II	U	C	8	0	0
2	Construct MO's of simple molecules based on Huckel method	PSO I	An	C	6	0	0
3	Study of aromaticity,antiaromaticity and homoaromaticity with MO description	PSO I	U	C	6	0	0
4	Acquire knowledge about basic concepts in the study of organic reaction mechanism	PSO II	U	C	6	0	0
5	Describe the factors affecting conformational stability of molecules	PSO I	An	F	6	0	0
6	Analyse the effect of conformation on the course and rate of reaction in various systems	PSO II	An	C	6	0	0
7	Evaluate optical and geometrical isomerism of organic compounds	PSO II	E	C	8	0	0
8	Summarise the chiral pool concept,Chiral auxiliaries and chira reagents	PSO II	U	P	8	0	0

Total hours of instruction 54

**Course Code : **VPCH1CO4

Course Title : THERMODYNAMICS, KINETICS AND CATALYSIS (3Credits, 54hrs)

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :
VPCH1CO4 – THERMODYNAMICS, KINETICS AND CATALYSIS (3 Credits, 54hrs)

Unit 1: Thermodynamics (9hrs)

Review of First and Second law of thermodynamics, Third law of thermodynamics, Need for third law, Nernst heat theorem, Apparent exceptions to third law, Applications of Third law, Determination of Absolute entropies, Residual entropy.

Thermodynamics of Solutions: Partial molar quantities, Chemical potential, Variation of chemical potential with temperature and pressure, Partial molar volume and its determination, Gibbs-Duhem equation, Thermodynamics of ideal and real gases and gaseous mixtures, Fugacities of gases and their determinations, Activity, Activity coefficient, standard state of substance (for solute and solvents), Duhem-Margules equation and its applications. Thermodynamics of ideal solutions, Phase equillibria : Applicaions to binary liquid system-separation of two miscible liquid-formation of azetropic mixture Non ideal solutions, Deviations from Raoult's law, Excess functions- excess free energy, excess entropy, excess enthalpy, excess volume.

Unit 2: Thermodynamics of Irreversible Processes (9 hrs).
Simple examples of irreversible processes, general theory of non-equilibrium processes, entropy production, the phenomenological relations, Onsager reciprocal relations, Vailidity and verification of Onsagar theoryapplication to the theory of diffusion, thermal diffusion, thermo-osmosis and thermo-molecular pressure difference, electro-kinetic effects, the Glansdorf-Pregogine equation.

Unit 3: Chemical Kinetics (9 hrs)
Kinetics of reactions involving reactive atoms and free radicals - Rice - Herzfeld mechanism and steady state approximation in the kinetics of organic gas phase decompositions (acetaldehyde & ethane); Kinetics of chain reactions – branching chain and explosion limits (H_2-O_2 reaction as an example); Kinetics of fast reactions-relaxation methods, molecular beams, flash photolysis; Solution kinetics: Factors affecting reaction rates in solution, Effect of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effects.

Unit 4: Molecular Reaction Dynamics (9 hrs)
Reactive encounters: Collision theory, diffusion controlled reactions, the material balance equation, Activated Complex theory – the Eyring equation, thermodynamic aspects of ACT; Comparison of collision and activated complex theories; The dynamics of molecular collisions – Molecular beams, principle of crossed-molecular beams; Potential energy surfaces - attractive and repulsive surfaces, London equation, Statistical distribution of molecular energies; Theories of unimolecular reactions - Lindemann's theory, Hinshelwood's modification, Rice -Ramsperger

and Kassel (RRK) model.

Unit 5: Surface Chemistry (9 hrs)

Adsorption: Adsorption isotherms, Langmuir's unimolecular theory of adsorption, BET equation, derivation, determination of surface area of adsorbents, heat of adsorption and its determination; Experimental methods for studying surfaces – SEM, TEM, and ESCA

Unit 6: Catalysis (9hrs)

Homogeneous catalysis–mechanism -Arrhenius intermediates and van't Hoff intermediates - acid base catalysis – specific and general acid catalysis – enzyme catalysis- Michaelis-Menten Mechanism- Auto catalysis - oscillating reactions – mechanisms of oscillating reactions (Lotko - Volterra, brusselator and oregonator) Heterogenous catalysis –adsorption and catalysis- unimolecular surface reactions – bimolecular surface reaction –Langmuir-Hinshelwood mechanism and Eley-Rideal mechanism – illustration using the reaction $2CO + O_2$ ---› $2CO_2$

References:

1. *P. Atkins & J. De Paula, Atkins's Physical Chemistry, 10/e, OUP, 2014*.

2 Keith J. Laidler, *Chemical Kinetics 3rd edn*., Pearson Education, 1987(Indian reprint 2008).

3. Steinfeld, Francisco and Hase, *Chemical Kinetics and Dynamics, 2nd edition,* Prentice Hall International . Inc

4. Santhosh K. Upadhyay, *Chemical Kinetics and Reaction Dynamics,* Springer, 2006.

5. Richard I. Masel, *Chemical Kinetics and Catalysis* , Wiley Interscience, 2001.

6. K.J.Laidler, J.H.Meiser and B. C. Sanctuary, *Physical Chemistry,* Houghton Mifflin Company, New York, 2003.

7. A.W. Adamson, *Physical Chemistry of surfaces*, 4th edition, Interscience, New York, 1982.

8. G. K. Vemulapalli, *Physical Chemistry*, Printice Hall of India.

9. M.K. Adam, *The Physics and Chemistry of surfaces* , Dover Publications

10. S. Glasstone, *Thermodynamics for chemists*, East-West 1973.

11. Rajaram and Kuriokose, *Thermodynamics,* East-West 1986

12. Pigoggine, *An introduction to Thermodynamics of irreversible processes*, Interscience

13. B.G. Kyle, *Chemical and Process Thermodynamics*, 2nd Edn, Prentice Hall of India

COURSE CODE : VPCH1CO4

COURSE: THERMODYNAMICS, KINETICS AND CATALYSIS (3 Credits, 54hrs)

Credits: 3

Instructors: Susan Samuel, Jidha K S **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Analyse third law of thermodynamics to determine absolute and residual entropy	PSO I	An	F	6	0	0
2	Acquire knowledge about thermodynamics of solutions,ideal,real gases and gaseous mixtures	PSO II	U	C	8	0	0
3	Generate idea about excess fun ctions such as excess free energy,excess entropy,excess enthalpy, excess volume	PSO I	U	C	6	0	0
4	Evaluate Validity and verification of Onsager theory and its application to theory of diffusion	PSO I	E	F	6	0	0
5	Summarise the kinectics of chain reactions,fast reactions and solution kinetics	PSO II	An	C	8	0	0
6	Understand molecular reaction dynamics using molecular beams	PSO II	U	P	6	0	0
7	Study Langmuir theory of adsorption,BET equation and experimental methods for topology analysis	PSO II	U	C	8	0	0
8	Compare homogenous and heterogenous catalysis	PSO I	E	F	6	0	0

Total hours of instruction 54

Department : Chemistry

Programme : M.Sc Chemistry

Semester : II

Course Code : VPCH2CO5

Course Title : APPLICATIONS OF QUANTUM MECHANICS ANFD GROUP THEORY
Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH2CO5-APPLICATIONS OF QUANTUM MECHANICS & GROUP THEORY(3Credits, 54hrs)

Unit 1: Approximation Methods in Quantum Mechanics (9hrs)
Many body problem and the need of approximation methods; Independent particle model; Variation method – variation theorem with proof, illustration of variation theorem using a trial function [e.g., x (a-x)] for particle in a 1D-box and using the trial function e^{-r2} for the hydrogen atom, variation treatment for the ground state of helium atom; Perturbation method – time-independent perturbation method (non-degenerate case only), illustration by application to particle in a ID-box with slanted bottom, perturbation treatment of the ground state of the helium atom.

Unit 2: Quantum Mechanics of Many-electron Atoms (9hrs)
Hartree Self-Consistent Field method for atoms; Spin orbitals for many electron atoms, symmetric and antisymmetric wave functions, Pauli's antisymmetry principle; Slater determinants; Hartree -Fock Self- Consistent Field (HF-SCF) method for atoms, Hartree -Fock equations (derivation not required) & the Fock operator; Roothan's concept of basis functions – Slater type orbitals (STO) and Gaussian type orbitals (GTO).<u>Slaters rule,rules for calculation of effective nuclear charge.STO's for He,C,and N</u>

Unit 3: Chemical bonding in diatomic molecule (9hrs)
Schrödinger equation for a molecule, Born – Oppenheimer approximation; Valence Bond (VB) theory – VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2; Molecular Orbital (MO) theory – MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules – Li_2, Be_2, C_2, N_2, O_2& F_2 and hetero nuclear diatomic molecules – LiH, CO, NO & HF, bond order, correlation diagrams, non-crossing rule; Spectroscopic term symbols for diatomic molecules; Comparison of MO and VB theories.

Unit 4: Chemical Bonding in polyatomic molecules (9hrs)
Hybridization – quantum mechanical treatment of sp, sp^2 & sp^3 hybridisation; Semi empirical MO treatment of planar conjugated molecules – Hückel Molecular Orbital (HMO) theory of ethylene, butadiene & allylic anion, charge distributions and bond
orders from the coefficients of HMO, calculation of free valence, HMO theory of aromatic hydrocarbons (benzene); formula for the roots of the Hückel determinantal equation, Frost -

Hückel circle mnemonic device for cyclic polyenes.

Unit 5: Applications of Group Theory to Molecular Spectroscopy (9hrs)

Molecular vibrations - symmetry species of normal modes of vibration, construction of cart, normal coordinates and drawings of normal modes (e.g., H_2O and NH_3), selection rules for IR and Raman activities based on symmetry arguments, determination of IR active and Raman active modes of molecules (e.g., H_2O, NH_3, CH_4 , SF_6), complementary character of IR and Raman spectra.

Spectral transition probabilities - direct product of irreducible representations and its use in identifying vanishing and non –vanishing integrals, transition moment integral and spectral transition probabilities, overlap integrals and conditions for overlap.

Electronic Spectra – electronic transitions and selection rules, Laporte selection rule for centro symmetric molecules.

Unit 6: Applications of Group Theory to Chemical Bonding (9hrs)

Hybridisation - Treatment of hybridization in BF_3 and CH_4, Inverse transformation and construction of hybrid orbitals. Molecular orbital theory – HCHO and H_2O as examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator, construction of SALC using proj ection operator, use of projection operator in constructing SALCs for the MOs in cyclopropenyl ($C_3H_3^+$) cation.

References (for Units 1 to 4)

1. F.L. Pilar, *Elementary Quantum Chemistry*, mcgraw-Hill, 1968.

2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc.,

3. I.N. Levine, *Student Solutions Manual for Quantum Chemistry 6th Edition*, Pearson Education Inc., 2009.

4. P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 4th Edition, Oxford University Press, 2005.

5. M.W. Hanna, *Quantum Mechanics in Chemistry*, 2nd Edition, W.A. Benjamin Inc., 1969.

6. Donald, A. Mcquarrie, *Quantum Chemistry*, University Science Books, 1983 (first Indian edition, Viva books, 2003).

7. Thomas Engel, *Quantum Chemistry & Spectroscopy*, Pearson Education, 2006.

8. J.P. Lowe, *Quantum Chemistry*, 2nd Edition, Academic Press Inc., 1993.

9. Horia Metiu, *Physical Chemistry–Quantum Mechanics*, Taylor & Francis, 2006.

10. A.K. Chandra, *Introduction to Quantum Chemistry*, 4th Edition, Tata mcgraw-Hill, 1994.

11. L. Pauling and E.B. Wilson, *Introduction to Quantum Mechanics*, mcgraw-Hill, 1935 (A good source book for many derivations).

12. R.L. Flurry, Jr., *Quantum Chemistry*, Prentice Hall, 1983.

13. R.K. Prasad, *Quantum Chemistry*, 3rd Edition, New Age International, 2006.

14. M.S. Pathania, *Quantum Chemistry and Spectroscopy (Problems & Solutions)*, Vishal Publications, 1984.

15. C.N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books Pvt. Ltd.,1998.

16. Jack Simons, *An Introduction to Theoretical Chemistry*, Cambridge University Press, 2003.

For Units 5&6

1. F.A.Cotton, *Chemical applications of Group Theory*, 3rd Edition, John Wiley &Sons Inc. 2003.

2. H. H. Jaffe and M. Orchin, *Symmetry in Chemistry,* John Wiley &Sons Inc., 1965.

3 .L.H. Hall, *Group Theory and Symmetry in Chemistry*, mcgraw Hill, 1969.

4.R. Mcweeny, *Symmetry: An Introduction to Group Theory and its Applications*,

Pergamon Press, London, 1963.

5. P.H. Walton, *Beginning Group Theory for Chemistry*, Oxford University Press Inc.,

Newyork, 1998.

6. Mark Ladd, *Symmetry & Group Theory in Chemistry*, Horwood 1998.

7. A. Salahuddin Kunju & G. Krishnan, *Group Theory & its Applications in Chemistry,*

PHI Learning Pvt. Ltd. 2010.

8. Arthur M Lesk, *Introduction to Symmetry & Group theory for Chemists*, Kluwer

Academic Publishers, 2004.

9. K.Veera Reddy, *Symmetry & Spectroscopy of Molecules 2nd Edn.*, New Age

International 2009.

10. A.W. Joshi, *Elements of Group Theory for Physicists*, New Age International

Publishers, 1997.

COURSE: APPLICATIONS OF QUANTUM MECHANICS ANFD GROUP THEORY

Credits: 3

Instructors: Susan Samuel,Anjali T R **Total hours: 54**
3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Analyse approximate methods of quantum mechanics.	PSO I	An	P	8	0	0
2	Summarise many electron system and antisymmetry principle.	PSO I	E	C	6	0	0
3	Compare the elementary concepts of MO and VB theories.	PSO I	An	F	8	0	0
4	Illustrate Huckel theory for conjugated pi-electron systems.	PSO I	E	P	6	0	0
5	Understand the hybridization in molecules.	PSO II	U	P	6	0	0
6	Construction of SALC using projection operator	PSO II	Ap	P	6	0	0
7	Classify atomic orbitals involved into symmetry species.	PSO I	E	F	6	0	0
8	Evaluate IR and RAMAN active modes of molecules	PSO II	Ap	P	8	0	0

Total hours of instruction 54

Course Code **:** VPCH2CO6

Course Title **: COORDINATION CHEMISTRY**

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH2CO6 - CO-ORDINATION CHEMISTRY (3Credits, 54hrs)

Unit 1: Stability of Co-ordination Compounds (9hrs)

Stereochemistry of coordination compounds. Stepwise and overall formation constants and the relationship between them. Trends in stepwise formation constants. Determination of binary formation constants by pH-metry and spectrophotometry. Stabilisation of unusual oxidation states. Ambidentate and macrocyclic ligands. Chelate effect and its thermodynamic origin. Macrocyclic and template effects.

Coordination compounds with special properties: stereochemically non-rigid and fluxional compounds.

Unit 2: Theories of Bonding in Coordination Compounds (9hrs)

Sidgwick`s electronic interpretation of coordination. The valence bond theory and its limitations. The crystal field and ligand field theories. Splitting of d-orbitals in octahedral, tetrahedral and square planar fields. Factors affecting crystal field splitting. Spectrochemical and nephelauxetic series. Racah parameters. Jahn-Teller effect. Molecular orbital theory-composition of ligand group orbitals. MO diagram of octahedral, tetrahedral and square planar complexes. π-bonding and molecular orbital theory.

Unit 3: Electronic Spectra and Magnetic Properties of Complexes (9hrs)

Spectroscopic ground state. Terms of d^n configurations. Selection rules for d-d transitions. Effect of ligand fields on RS terms in octahedral and tetrahedral complexes. Orgel diagrams. Calculation of D_q, B and β parameters. Tanabe-Sugano diagrams. Charge transfer spectra.

Types of magnetic properties-Paramagnetism and diamagnetism. Curie and Curie-Weiss laws.The μ_J , μ_{L+S} and μ_S expressions. Orbital contribution to magnetic moment and its quenching. Spin-orbit coupling. Temperature independent paramagnetism. Antiferromagnetism-typesand exchange pathways. Determination of magnetic moment by Gouy method

Unit 4: Characterization of Coordination Complexes (9hrs)

complexes. ESR spectra – application to copper complexes. NMR spectroscopy for structural studies of diamagnetic metal complexes from chemical shift and spin- spin coupling. Mossbauer spectroscopy- the Mossbauer effect, hyperfine interactions (qualitative treatment). Application to iron and tin compounds.

Unit 5: Reaction Mechanism of Metal Complexes (9hrs)

Ligand substitution reactions. Labile and inert complexes. Rate laws. Classification of mechanisms-D, A and I mechanisms. Substitution reactions in octahedral complexes. The Eigen-Wilkins Mechanism. Fuoss-Eigen equation. Aquation and base hydrolysis-mechanism.

Substitution reactions in square planar complexes. The trans effect-Applications and theories of trans effect. The cis effect.

Unit 6: Redox and Photochemical Reactions of Complexes (9hrs)

Classification of redox reaction mechanisms. Outer sphere and inner sphere mechanisms. Marcus equation. Effect of the bridging ligand. Methods for distinguishing outer- and inner-sphere redox reactions.

Photochemical reactions of metal complexes- Prompt and delayed reactions. Exited states of metal complexes- Interligand, ligand field, charge transfer and delocalized states.. Photosubstitution-Prediction of substitution lability by Adamson`s rules. Photoaquation. Illustration of reducing and oxidizing character of $[Ru(bipy)_3]^{2+}$ in the excited state. Infra-red spectra of metal complexes, group frequency concept, changes in ligand vibrations on coordination- metal ligand vibrations.

References:

1. N.n.greenwood and a.earnshaw, *chemistry of elements*, *2/e*, butterworth-Heinemann, 2005.

2 j.e.huheey, e.a.keiter, r.l.keiter and o.k.medhi, *inorganic chemistry, principles Of structure* and *reactivity*, pearson education, 2006.

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4. D.f.shriver, p.w.atkins, *inorganic chemistry,*oxford university press, 2002

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8. B.douglas, d.mcdaniel, j.alexander, *concepts and models of inorganic Chemistry,*wiley student edition, 2006.

9. A.w.adamson and p.d.fleischauer, *concepts of inorganic photochemistry, wiley.*

10. F.a.cotton and g.wilkinson, *advanced inorganic chemistry*, wiley.

11. A.earnshaw, *introduction to magnetochemistry, academic press, 1968.*

12. R.l.dutta and a.shyamal, *elements of magnetochemistry*, s.chand and co. 1982.

13. A.e. martell, *coordination chemistry, vol. I*

14. R.s. drago, *physical methods in inorganic chemistry*, affiliated east- west press Pvt. Ltd., 1977

COURSE: COORDINATION CHEMISTRY **Credits: 3**

Instructors: Anjali T R, Megha C.B **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Understand the basic factors the affect the stability of coordination compounds.	PSO I	U	C	6	0	2
2	Study the bonding in coordination complexes by VBT,CFT,MOT	PSO I	An	C	6	0	0
3	Draw the MO diagram of several complexes	PSO I	Ap	F	6	0	0
4	Acquire knowledge about Orgel diagram, Tanabe –Sugano diagram	PSO I	Ap	P	6	0	0
5	Determine the magnetic properties of coorination complexes	PSO I	U	C	6	0	0
6	Characterize a given coordination complex by various spectroscopic techniques	PSO III	Ap	P	6	0	0
7	Evaluate actual reaction mechanisms exhibited by metal complexes	PSO II	E	F	6	0	2
8	Compare outer sphere and inner sphere redox reactions in coordination complexes	PSO I	U	P	8	0	0

Total hours of instruction	50	4

Course Code **:** VPCH2CO7

Course Title **: REACTION MECHANISM IN ORGANIC CHEMISTRY**
Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH2CO7 - REACTION MECHANISM IN ORGANIC CHEMISTRY(3 Credits, 54hrs)

Unit 1: Aliphatic and Aromatic Substitutions (9 hrs)

Nucleophilic Aliphatic Substitution: Mechanism and Stereochemistry of S_N2 and S_N1 reactions. Ion pair mechanism. The effect of substrate structure, reaction medium, nature of leaving group and nucleophile on S_N2 and S_N1 reactions. S_Ni and neighboring group mechanism. SET mechanism. Allylic and bezylic substitutions. Ambident nucleophiles and substrates regioselectivity.

Electrophilic Aliphatic Substitution: Mechanism and stereochemistry of S_E1, S_E2 (front), S_E2 (back) and S_Ei reactions. The effect of substrate structure, leaving group and reaction medium on S_E1 and S_E2 reactions.

Electrophilic Aromatic Substitution: Arenium ion mechanism, substituent effect on reactivity in mono and disubstituted benzene rings, *ortho/para* ratio, *Ipso* substitution. Relationship between reactivity and selectivity. Nucleophilic Aromatic substitution: Addition-elimination (S_NAr) mechanism, elimination-addition (benzyne) mechanism, *cine* substitution, S_N1 and $S_{RN}1$ mechanism. The effect of substrate structure, nucleophile and leaving group on aromatic nucleophilic substitution.

Unit 2: Addition & Elimination Reactions and Reactive Intermediates (9hrs)

(i) Addition and Elimination Reactions (6 hrs)

Mechanistic and stereochemical aspects of addition to C=C involving electrophiles, nucleophiles and free radicals. Effect of substituents on rate of addition, orientation of addition, addition to conjugated systems and cyclopropane rings, Michael reaction.

Mechanistic and stereochemical aspects of E1, E1cB and E2 eliminations. The effect of substrate structure, base, leaving group and reaction medium on elimination reactions. Saytzev *vs* Hofmann elimination, α-elimination, pyrolytic *syn* elimination (E*i*) and conjugate eliminations. Competition between substitution and elimination reactions, basicity *vs* nucleophilicity. Extrusion reactions-extrusion of N_2, CO and CO_2.

(ii) Reactive Intermediates (3 hrs)
Reactive Intermediates: Generation, geometry, stability and reactions of carbonium ions and

carbanions, free radicals, carbenes, nitrenes and benzynes

Unit 3: Chemistry of Carbonyl Compounds (9hrs)

(i) Reactions of Carbon-heteromultiple Bonds (7 hrs)

Reactivity of carbonyl compounds toward addition, mechanistic aspects of hydration, addition of alcohols, and condensation with nitrogen nucleophiles to aldehydes and ketones. Addition of organometallic reagents- Grignard reagents- organozinc, organocopper and organolithium reagents- to carbonyl compounds. Aldol, Perkin, Claison, Dieckmann, Stobbe and benzoin condensation. Darzen's, Knoevenagel, Reformatsky, Wittig, Cannizaro, Mannich and Prins reactions. MPV reduction and Oppenauer oxidation.

Addition to carbon-nitrogen multiple bond: Ritter reaction and Thorpe condensation. Hydrolysis, alcoholysis and reduction of nitriles.

(ii) Esterification and Ester Hydrolysis (2hrs): Mechanisms of ester hydrolysis and esterification, Acyl-oxygen and alkyl oxygen cleavage.

Unit 4: Pericyclic Reactions (9 hrs)

Phase and symmetry of molecular orbitals, FMOs of ethylene, 1,3-butadiene, 1,3,5- hexatriene, allyl and 1,3-pentadienyl systems. Pericyclic reactions: electrocyclic, cycloaddition, sigmatropic, chelotropic and group transfer reactions. Theoretical models of pericyclic reactions: TS aromaticity method (Dewar-Zimmerman approach), FMO method and Correlation diagram method (Woodward-Hoffmann approach). Woodward- Hoffmann selection rules for electrocyclic, cycloaddition and sigmatropic reactions. Stereochemistry of Diels-Alder reactions and regioselectivity. Cope and Claison rearrangements. Stereochemistry of cope rearrangement and valence tautomerism.

Unit 5: Photochemistry of Organic Compounds (9 hrs)

Photochemical excitation of molecules, spin multiplicity, Jablonski diagram, inter system crossing,energy transfer:Stern-Volmer equation. photosensitization and quenching. Photochemistry of carbonyl compounds: Norrish type-I cleavage of acyclic, cyclic and β, γ-unsaturated carbonyl compounds, β- cleavage, γ- hydrogen abstraction: Norrish type-II cleavage, photo reduction, photoenolization. Photocyclo-addition of ketones with unsaturated compounds: Paterno-Büchi reaction, photodimerisation of α, β-unsaturated ketones, Photo rearrangemets: Photo –Fries, di-π- methane, lumiketone, oxa di-π-methane rearrangements. Barton and Hoffmann-Loeffler- Freytag reactions. Photo isomerisation and dimerisation of alkenes, photo isomerisation of benzene and substituted benzenes, photooxygenation.

Unit 6: Chemistry of Natural Products (9 h)

Chemical classification of natural products. Classification of alkaloids based on ring structure, isolation and general methods of structure elucidation based on degradative reactions. Structures

of atropine and quinine. Terpenoids - Isolation and classification of terpenoids, structure of steroids classification of steroids. Woodward synthesis of
cholesterol, conversion of cholesterol to testosterone. Total synthesis of Longifolene,

Reserpine, Cephalosporin, Flavones and Isoflavones- synthesis only.

References:

1. M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 6/e, John Wiley & Sons, 2007.
2. F. A. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A & B*, 5/e, Springer, 2007.
3. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2005.
4. T. H. Lowry and K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3/e Addison-Wesley, 1998.
5. R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3/e, CRC Press, 1998.
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9. J. Sing and J. Sing, *Photochemistry and Pericyclic Reactions*, 3/e, New Age International, 2012.
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11. M. B. Smith, *Organic Chemistry: An Acid Base Approach*, CRC Press, 2010.
12. T. Okuyama and H. Maskill, *Organic Chemistry A Mechanistic Approach*, Oxford University Press, 2014.
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14. T. Landbery, *Strategies and Tactics in Organic Synthesis*, Academic Press, London,1989.
15. E. Corey and i.m. chang, *logic of chemical synthesis*, john wiley, new york, 1989.
16. I. L. Finar, *organic chemistry vol 2: stereochemistry and the chemistry of natural Products*, 5/e, pearson, 2006.
17. N. R.krishnaswamy, *chemistry of natural products: a laboratory hand book*, 2/e, Universities press

COURSE: REACTION MECHANISM IN ORGANIC CHEMISTRY **Credits: 3**

Instructors: Susan Samuel, Megha C.B **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Understand aliphatic and aromatic,nucleophilic and electrophilic substitution with mechanism.	PSO II	U	C	6	0	2
2	Study the reaction mechanism involving addition and eliminaton reaction with electrophiles and nucleophiles.	PSO II	U	C	6	0	2
3	Compare the stability , geometry and rections of rective intermediates.	PSO I	E	F	4	0	0
4	Analyse several nucleophilic reactions of carbonyl compounds.	PSO II	An	F	6	0	2
5	Understand the different mechanisms of ester hydrolysis and evidence.	PSO II	R	C	6	0	2
6	Apply the basic concepts and theory of pericyclic reactions.	PSO I	U	P	6	0	0
7	Summaries the principles and applications of photochemicals in organic chemistry	PSO I	An	F	6	0	0

8	Compare and classify natural products	PSO I	U	C	6	0	0
	Total hours of instruction				46		8

**Course Code : ** VPCH2CO8

Course Title : ELECTROCHEMISTRY,SOLIDSTATE CHEMISTRY AND STATISTICAL THERMODYNAMICS

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH2CO8 - ELECTROCHEMISTRY, SOLID STATE CHEMISTRY AND STATISTICAL THERMODYNAMICS (3 Credits, 54hrs)

Unit 1: Ionic Interaction & Equilibrium Electrochemistry (9hrs)

The nature of electrolytes, Ion activity, Ion-ion and ion-solvent interaction, The electrical potential in the vicinity of an ion, Electrical potential and thermodynamic functions. The Debye-Hückel equation,Limiting and extended forms of the Debye-Hückel equation, Applications of the Debye-Hückel equation for the determination of thermodynamic equilibrium constants and to calculate the effect of ionic strength on ion reaction rates in solution

Origin of electrode potentials-half cell potential-standard hydrogen electrode, reference electrodes- electrochemical series, applications- cell potential, Nernst equation for electrode and cell potentials, Nernst equation for potential of hydrogen electrode and oxygen electrode-thermodynamics of electrochemical cells, efficiency of electrochemical cells and comparison with heat engines-primary cells (Zn, MnO_2) and secondary cells (lead acid, Ni-Cd and Ni-MH cells), electrode reactions, potentials and cell voltages, advantages and limitations three types of secondary cells.
-fuel cells; polymer electrolyte fuel cell (PEMFCs), alkaline fuel cells (AFCs), phosphoric acid fuel cells (PAFCs), direct methanol fuel cells, electrode reactions and potentials, cell reactions and cell voltages, advantages and limitations of four types of fuel cells

Unit 2: Dynamic Electrochemistry (9hrs)

Electrical double layer-electrode kinetics of electrode processes, the Butler-Volmer equation-The relationship between current density and overvoltage, the Tafel equation. Polarization - electrolytic polarization, dissolution and deposition potentials, concentration polarization; Overvoltage: hydrogen overvoltage and oxygen overvoltage: decomposition potential and overvoltage, individual electrode over voltages and its determination-metal deposition over voltage and its determination- theories of hydrogen overvoltage, the catalytic theory, the slow discharge theory, the electrochemical theory. Principles of polarography -dropping mercury electrode, the half wave potential.

UNIT 3: Solid State – I (9hrs)

Crystal symmetry: Symmetry elements and symmetry operations, mathematical proof for the non-existence of 5-fold axis of symmetry, crystal systems, Bravais lattices and crystal classes, Crystallographic point groups - Schönflies & Hermann–Mauguin notations, Stereographic projections of the 27 axial point groups, translational symmetry elements & symmetry operations - screw axes and glide planes, introduction to space groups.

Bragg's law and applications, lattice planes and miller indices, *d*-spacing formulae, crystal densities and unit cell contents,

Imperfections in solids - point, line and plane defects, non-stoichiometry.

UNIT 4: Solid State – II (9hrs)

Electronic structure of solids – free electron theory, band theory & Zone theory, Brillouin zones; Electrical properties - electrical conductivity, Hall effect, dielectric properties, piezo electricity, ferro-electricity and ionic conductivity; Superconductivity-Meissner effect, brief discussion of Cooper theory of superconductivity; Optical properties - photo conductivity, luminescence, colour centers, lasers, refraction & birefringence; Magnetic properties - diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism & ferrimagnetism; Thermal properties - thermal conductivity & specific heat

Unit 5: Statistical Thermodynamics- I (9hrs)

Fundamentals – concept of distribution, thermodynamic probability and most probable distribution, ensembles, statistical mechanics for systems of independent particles and its importance in chemistry, thermodynamic probability & entropy, idea of microstates and macrostates, statistical weight factor (g), Sterling approximation, Maxwell-Boltzman statistics. The molecular partition function and its relation to the thermodynamic properties, derivation of third law of thermodynamics, equilibrium-constant & equi-partition principle in terms of partition functions, relation between molecular & molar partition functions, factorisation of the molecular partition function into translational, rotational, vibrational and electronic parts, the corresponding contributions to the thermodynamic properties; Evaluation of partition functions and thermodynamic properties for ideal mono-atomic and diatomic gases.

Unit 6: Statistical Thermodynamics- II (9hrs)

Heat capacities of solids - classical and quantum theories, Einstein's theory of atomic crystals and Debye's modification.

Quantum Statistics: Bose - Einstein distribution law, Bose-Einstein condensation, application to liquid helium; Fermi - Dirac distribution law, application to electrons in metals; Relationship between Maxwell-Boltzman, Bose-Einstein, and Fermi-Dirac statistics.heat capacity of mono and diatomic gases. Ortho and para hydrogen and the mixture of the two viz:O-H_2 and P-H_2.

REFERENCES:

For units 1-4

1. D. R. Crow, *principles and applications of electrochemistry*, chapman and hall London, 1979.
2. J.o.m. bockris and a.k.n. reddy, *modern electrochemistry, vol. I and ii*, Kluwer academic / plenum publishers, 2000.
3. Carl. H. Hamann, a. Hamnett, w.vielstich, *electrochemistry 2nd edn.*, wiley-Vch, 2007.
4. Philip h reiger, *electrochemistry 2nd edn.*, chapman & hall, 1994.
5. Praveen tyagi, *electrochemistry*, discovery publishing house, 2006.
6. D.a. mcinnes, *the principles of electrochemistry*, dover publications, 1961.
7. L.v. azaroff, *introduction to solids*, mcgraw hill, ny, 1960.
8. A.r. west, *basic solid state chemistry 2nd edn.*, john wiley & sons, 1999.
3. A.r. west, *solid state chemistry & its applications,* john wiley & sons, 2003 (reprint 2007).
4. Charles kittel, *introduction to solid state physics*, *7th edn*, john wiley & Sons, 2004 (reprint 2009).
5. Mark ladd, *crystal structures: lattices & solids in stereo view*, horwood, 1999.
6. Richard tilley, *crystals & crystal structures*, john wiley & sons, 2006.
7. C. Giacovazzo (ed.) *Fundamentals of crystallography 2nd edn.*, oxford uty. Press, 2002.
8. Werner massa, *crystal structure determination 2nd edn*., springer 2004.
9. N.b. hanna, *solid state chemistry,* prentice hall

For units 5 & 6

1. G.s. rush brooke, *statistical mechanics,* oxford university press.
2. T.l. hill, *introduction to statistical thermodynamics*, addison wesley.
3. K. Huary, *statistical mechanics, thermodynamics and kinetics* , john wiley.
4. O.k.rice, *statistical mechanics, thermodynamics and kinetics*, freeman and co.
5. F.c. andrews, *equilibrium statistical mechanics* , john wiley and sons, 1963.
6. M.c. guptha, *statistical thermodynamics* , wiley eastern ltd., 1993.

COURSE: ELECTROCHEMISTRY,SOLIDSTATE CHEMISTRY AND STATISTICAL THERMODYNAMICS

Credits: 3

Instructors: Anjali T R, Megha C.B **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Describe Debye-Huckel equation – limiting and extended forms.	PSO I	U	C	8	0	0
2	Study the efficiency of electrochemical cells with heat engines.	PSO I	An	C	6	0	0
3	State the different theories of hydrogen overvoltage	PSO I	An	F	6	0	0
4	Acquire knowledge about polarography and DME	PSO I	U	F	6	0	0
5	Evaluate the crystal structures , Bragg's law and applications	PSO I	U	C	6	0	0

6	Compare electrical,thermal,magnetic and optical properties of solid.	PSO I	An	C	6	0	0
7	Evaluate partition functions and their relation to thermodynamic quantities	PSO I	E	F	8	0	0
8	Compare M-B,B-E and F-D statistics	PSO I	U	C	8	0	0

Total hours of instruction 54

Department : Chemistry

Programme : M.Sc Chemistry

Semester : III

Course Code : VPCH3CO9

Course Title : MOLECULAR SPECTROSCOPY (3 Credits, 54hrs)

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH3CO9- MOLECULAR SPECTROSCOPY (3 Credits, 54hrs)

Unit1: Basic Aspects and Microwave Spectroscopy - ***Theory only*** **(9hrs)**

Electromagnetic radiation & it's different regions, Interaction of matter with radiation and its effect on the energy of a molecule, Factors affecting the width and Intensity of Spectral lines- transition moment integral.

Microwave spectroscopy **-** Rotation spectra of diatomic and poly atomic molecules - rigid and non-rigid rotator models, asymmetric, symmetric and spherical tops, isotope effect on rotation spectra, Stark effect, nuclear and electron spin interactions, rotational transitions and selection rules, determination of bond length using microwave spectral data. Centrifugal distortion constant.

Unit 2: Infrared, Raman and Electronic Spectroscopy - ***Theory only*** **(9hrs)**

Vibrational spectroscopy -Normal modes of vibration of a molecule; Vibrational spectra of diatomic molecules, anharmonicity, Morse potential, fundamentals, overtones, hot bands, combination bands, difference bands; Vibrational spectra of polyatomic molecules; Vibration-rotation spectra of diatomic and polyatomic molecules, spectral branches -P, Q & R branches.

Raman spectroscopy **–**Classical and Quantum theory of Raman effect Pure rotational & pure vibrational Raman spectra, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle;
Electronic Spectroscopy- Characteristics of electronic transitions – Vibrational coarse structure, intensity of electronic transitions, Franck - Condon principle, types of electronic transitions; Dissociation and pre-dissociation; Ground and excited electronic states of diatomic molecules; Electronic spectra of polyatomic molecules; Electronic spectra of conjugated molecules;Photo-electron spectroscopy: principle and technique of PES and Ultra-Violet PES.

Unit 3: Magnetic Resonance Spectroscopy - ***Theory only*** **(9hrs)**

NMR: Quantum mechanical description of Energy levels-Population of energy-Transition probabilities using ladder operators-Nuclear shielding- Chemical shift- Spin-Spin coupling and splitting of NMR signals- Quantum mechanical Description- AX and AB NMR pattern-Effect of Relative magnitudes of J (Spin-Spin coupling) and Chemical Shift on the spectrum of AB type molecule. Karplus relationship.- Nuclear Overhauser Effect- FT NMR- Pulse sequence for T1 and T2 (Relaxation) measurements. 2D NMR COSY

Electron Spin Resonance: Theory and measurement technique, anisotropy in g value, causes of anisotropy. g factor-hyperfine interaction-Mc Connell Relation-Equivalent and non equivalent nucleus- g anisotropy- Zero field splitting -Kramer's theorem.Applications of ESR technique.
Mossbauer Spectroscopy: The Mossbauer effect, hyperfine interactions, isomer shift, electric quadruple and magnetic hyperfine interactions.

UNIT 4: Electronic & Vibrational Spectroscopy in Organic Chemistry (9hrs)

UV-Visible spectroscopy: Factors affecting the position and intensity of electronic absorption bands – conjugation, solvent polarity and steric parameters. Empirical rules for calculating λ_{max} of dienes, enones and benzene derivatives.

Optical Rotatory Dispersion and Circular Dichroism: Linearly and circularly polarized lights, circular birefringence, elipticity and circular dichroism, ORD and Cotton effect. Octant rule and Axial haloketone rule for the determination of conformation and configuration of 3-methyl cyclohexanone and *cis*- and *trans*-decalones. CD curves.
Infrared Spectroscopy: Functional group and finger print regions, Factors affecting vibrational frequency: Conjugation, coupling, electronic, steric, ring strain and hydrogen bonding. Important absorption frequencies of different class of organic compounds- hydrocarbons, alcohols, thiols, carbonyl compounds, amines, nitriles.

UNIT 5: NMR Spectroscopy in Organic Chemistry (9hrs)

^{1}HNMR: Chemical shift, factors influencing chemical shift, anisotropic effect. Chemical shift values of protons in common organic compounds, Chemical, magnetic and stereochemical equivalence. Enantiotopic, daisteriotopic and homotopic protons. Protons on oxygen and nitrogen. Quadrapole broadening. Spin –spin coupling, types of coupling. Coupling constant, factors influencing coupling constant, effects of chemical exchange, fluxional molecules, hindered rotation on NMR spectrum, First order and non first order nmr spectra, Simplification of NMR spectra: double resonance, shift reagents, increased field strength, deuterium labelling. NOE spectra, heteronuclear coupling. Introduction to COSY, HMBC, HMQC spectra.

^{13}CNMR: General considerations, comparison with PMR, factors influencing carbon chemical shifts, carbon chemical shifts and structure-saturated aliphatics, unsaturated aliphatics, carbonyls, and aromatics. Off-resonance and noise decoupled spectra, Introduction to DEPT, INEPT, INADEQUATE.

UNIT 6: Mass Spectrometry and Spectroscopy for Structure Elucidation (9hrs)

*Mass Spectrometry**:*** Basic concept of EIMS. Molecular ion and meta stable ion peaks, Isotopic peaks. Molecular weight and molecular formula. Single and multiple bond cleavage, rearrangements -McLafferty rearrangements. Fragmentation pattern of some common organic compounds – saturated and unsaturated hydrocarbons, ethers, alcohols, aldehydes and ketones, amines and amides. High resolution mass spectrometry, index of hydrogen deficiency, Nitrogen rule and Rule of Thirteen. Ionization techniques. FAB spectra.

Structural determination of organic compounds using spectroscopic techniques (Problem solving approach)

References: for units 1, 2 & 3:

1. G.m. barrow, *introduction to molecular spectroscopy*, mcgraw hill, 1962.

2. C.n. banwell & e. M. Mccash, *fundamentals of molecular spectroscopy*, tata mcgraw Hill,new delhi, 1994.

3. Thomas engel, *quantum chemistry & spectroscopy*, pearson education, 2006.

4. P. Atkins & j. De paula, *atkins's physical chemistry,* 8th edition, w.h. freeman & co., 2006.

5. D.a. mcquarrie and j.d. simon, *physical chemistry - a molecular approach*, university Science books, 1997.

6. D.n. sathyanarayana, *electronic absorption spectroscopy and related techniques*, Universitypress, 2000.

7. R.s. drago, *physical methods for chemists*, second edition, saunders college publishing 1977 (for nmr and epr, mossbauer)

8. Gunther, nmr spectroscopy: basic principles, concepts and applications in chemistry, 2/e, – john wiley

9. Ferraro, nakamoto and brown, introductory raman spectroscopy, 2/e, academic press, 2005.

For units 4, 5 & 6

1. Lambert, organic structural spectroscopy, 2/e,—pearson

2. Silverstein, spectrometric identification of organic compounds, 6/e,—john wiley

3. Pavia, spectroscopy, 4/e, – cengage

4. Jag mohan, organic spectroscopy: principles and applications, 2/e,—narosa

5. Fleming, spectroscopic methods in organic chemistry, 6/e, — mcgraw-hill

6. P s kalsi, spectroscopy of organic compounds, new age international, 2007

7. William kemp, organic spectroscopy**, 3e,** palgrave, 2010

COURSE: MOLECULAR SPECTROSCOPY **Credits: 3**

Instructors: **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Understand the basic fundamentals of microwave spectroscopy	PSO I	U	C	6	0	0
2	Analyse the vibrational spectra of polyatomic molecules	PSO II	An	P	6	0	0
3	Compare the classical and quantum theory of Raman effect	PSO I	C	C	6	0	0
4	Evaluvate kramers theorem in ESR spectroscopy	PSO I	E	P	6	0	0
5	Analyse Nuclear Overhauser Effect in FTNMR spectroscopy	PSO I	An	P	8	0	0
6	Understand the basic principles and applications of Mossbauer spectroscopy	PSO I	U	C	8	0	0
7	Analyse the structure of organic compounds by spectrometric methods	PSO II	An	P	8	0	0
8	Understand the basic principles of EIMS	PSO I	U	C	6	0	0

Total hours of instruction

**Course Code : ** VPCH3CO10
Course Title : ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY (3Credits, 54h)

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH3C10 - ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY (3Credits, 54h)

Unit 1: Introduction to Organometallic Chemistry (9hrs)

Classification and nomenclature. Alkyls and aryls of main group metals. Organometallic compounds of transition metals. The 18-electron rule-electron counting by neutral atom method and oxidation state method. The 16-electron rule.

Metal carbonyls- Synthesis, structure, bonding and reactions. Nytrosyl, dihydrogen and dinitrogen complexes. Transition metal to carbon multiple bond-metal carbenes and carbines.

Unit 2: Organometallic Compounds of Linear and Cyclic π-Systems (9hrs)

Transition metal complexes with linear π- systems-Hapticity. Sythesis , structure,bonding and properties of complexes with ethylene,allyl,butadiene and acetylene. Complexes of cyclic π-systems-Synthesis,structure,bonding and properties of complexes with cyclobutadiene, $C_5H_5^-$

C_6H_6, $C_7H_7^+$ and $C_8H_8^{2-}$. Fullerene complexes. Fluxional organometallics.

Unit 3: Organometallic Reactions and Catalysis (9hrs)

Organometallic reactions- ligand dissociation and substitution- Oxidative addition and reductive elimination.Insertion reactions involving CO and alkenes. Carbonylation by Collman`s reagent. Electrophilic and Nucleophilic attack on coordinated ligand.

Homogeneous and heterogeneous catalysts.

Homogeneous catalysis by organometallic compounds: Hydrogenation by Wilkinson`s catalyst, Hydroformylation, Wacker process, Monsanto acetic acid process, Cativa process and olefin metathesis.

Heterogeneous catalysis by organometalic compounds: Ziegler-Natta polymerizations, Fischer-Tropsch process and water gas shift reaction.

Unit 4: Metal Clusters (9hrs)

Metal-Metal bond and metal clusters. Bonding in metal-metal single,double,triple and quadruple bonded non-carbonyl clusters. Carbonyl clusters-electron count and structure of clusters. Wade-Mingos-Lauher rules. Structure and isolobal analogies. Carbide clusters. Polyatomic Zintl anions and cations. Chevrel phases.

Unit 5: Bioinorganic Chemistry-I (9hrs)

Occurrence of inorganic elements in biological systems- bulk and trace metal ions.
Thermodynamic and kinetic aspect of stability. Coordination sites in biologically important ligands. Ion transport across membranes. Role of alkali metal ions in biological systems. The sodium/potassium pump. Structural role of calcium. Storage and transport of metal ions- ferritin, transferrin and siderophores. Oxygen transport by heme proteins-hemoglobin and myoglobin-structure of the oxygen binding site-nature of heme-dioxygen binding-cooperativity. Hemerythrin and hemocyanin,hemovanadins.

Unit 6: Bioinorganic Chemistry-II (9hrs)

Metallo enzymes and electron carrier metallo proteins. Iron enzymes: Cytochrome P-450, catalase and peroxidase.Copper enzymes: Oxidase, superoxide dismutase and tyrosinase. Lewis acid role of Zn(II) and Mn(II) containing enzymes. Carboxypeptidase.role of Mg(II) containing enzymes. Vitamin B_{12} and coenzymes.Chlorophil II- Photosystem I and II. Nitrogen fixation-Nitrogenases. Anticancer drugs.

References:

1. N.n. greenwood and a.earnshaw, *chemistry of elements,* 2/e, elsevier butterworth-Heinemann, 2005.
2. J.e.huheey, e.a.keiter, r.l.keiter. O.k.medhi, *inorganic chemistry, principles of structure And reactivity,* pearson education, 2006.
3. G.l.miessler, d.a.tarr, *inorganic chemistry,* pearson, 2010.
4. D.f.shriver, p.w.atkins, *inorganic chemistry,* oxford university press, 2002
5. William w porterfield, *inorganic chemistry-a unified approach,* academic press, 2005.
6. Keith f purcell, john c kotz, *inorganic chemistry,* cengage learning, 2010.
7. James e house, *inorganic chemistry,* academic press, 2008.
8. B.douglas, d.mcdaniel, j.alexander, *concepts and models of inorganic chemistry,* wiley Student edition, 2006.
9. F.a.cotton and g.wilkinson, *advanced inorganic chemistry,* wiley.
10. R.c.mehrothra and a.singh, *organometallic chemistry, a unified approach, w*iley eastern.
11. P.powell, *principles of organometallic chemistry, elbs.*
12. B.d.gupta and a.j.elias, *basic organometallic chemistry, concepts, synthesis and Applications,* universities press, 2010.
13. Piet w.n. m.van leeuwen, *homogeneous catalysis*, springer, 2010.
14. S.j. lippard and j.m.berg, *principles of bioinorganic chemistry,* university science books.
15. I. Bertini, h.b. grey, s.j. lippard and j.s.valentine, *bioinorganic chemistry, viva books*

COURSE: ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

Credits: 3

Instructors: **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Evaluate 18 and 16 electron rule by neutral atom method and oxidation state method	PSO I	E	F	6	0	0
2	Acquire knowledge about synthesis,structure,bonding and reactions of metal carbonyls,nitrosyl,dihydrogen and dinitrogen complexes	PSO II	U	C	8	0	0
3	Study organometallic compounds of linear and cyclic pi systems	PSO I	U	C	6	0	0
4	Understand about oxidative addition,reductive elimination,insertion reactions	PSO II	U	C	8	0	0
5	Compare homogenous and heterogenous catalysis by organometallic compounds	PSO II	E	C	8	0	0
6	Analyse metal-metal bond and metal clusters	PSO I	An	C	6	0	0
7	Describe oxygen transport by heme proteins	PSO II	An	P	6	0	0
8	Summaries metallo enzymes and electron carrier metallo proteins	PSO I	U	F	6	0	0

Total hours of instruction

**Course Code : ** VPCH3CO11

Course Title : REAGENTS &TRANSFORMATIONS IN ORGANIC CHEMISTRY (3Credits, 54h)

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH3C11-REAGENTS &TRANSFORMATIONS IN ORGANIC CHEMISTRY (3Credts, 54hrs)

Unit 1: Oxidations (9hrs)

Oxidation of alcohols to carbonyls using DMSO, oxoammonium ions and transition metal oxidants (chromium, manganese, iron, ruthenium). Epoxydation of alkenes by peroxy acids, Sharpless asymmetric epoxidation, Jacobsen epoxidation, dihydroxylation of alkenes using permanganate ion and osmium tetroxide, Prévost and Woodward dihydroxylations, Sharpless asymmetric dihydroxylation. Allylic oxidation with CrO_3-Pyridine reagent. Oxidative cleavage of alkenes to carbonyls using O_3. Oxidative decarboxylation, Riley reaction, Baeyer-Villiger oxidation, Dess- Martin oxidation, Swern oxidation, hydroboration-oxidation.

Unit 2: Reductions (9hrs)

Catalytic hydrogenation of alkenes and other functional groups (heterogeneous and homogeneous), Noyori asymmetric hydrogenation, hydrogenolysis. Liquid ammonia reduction with alkali metals. Metal hydride reductions. Reduction of carbonyl group with hydrazine, p-tosylhydrazine, diimide and semicarbazide. Clemmensen reduction, Birch reduction. Wolff-Kishner reduction, Bouveault- Blanc reduction, MPV reduction, hydroboration, Pinacol coupling, McMurry coupling, Shapiro reaction.

Unit 3: Synthetic Reagents (9 hrs)

Synthetic applications of Crown ethers, β-cyclodextrins, PTC, ionic liquids, Baker's yeast, NBS, LDA, $LiAlH_4$, $LiBH_4$, DIEA, BuLi, diborane, 9-BBN, t-butoxycarbonylchloride, DCC, Gilman’s reagent, lithium dimethyl cuprate, tri-n-butyltinhydride, 1,3-dithiane, trimethyl silyl chloride, $Pb(OAc)_4$, ceric ammonium nitrate, DABCO, DMAP, DBU, DDQ, DEAD and Lindlar catalyst in organic synthesis.

Unit 4: Formation of Carbon-carbon bond(9 hrs)

Carbon-carbon bond formation via electrophillic and nucleophillic carbon species.base catalysed condensations, Mannich base as intermediates in organic synthesis, four centre reaction-Diel’s Alder reaction, 1,3-dipolar additions.

Unit 5: Chemistry of Heterocyclic Compounds (9 hrs)

Aromatic and nonaromatic heterocyclics. structure, synthesis and reactions of a few heterocyclics-aziridine, oxirane, azetidine, pyrrole, furan, thiophene, indole, pyridine, quinoline, imidazole, oxazole, pyrazole, and thiazole. synthesis of uracil, thymine, cytosine, adenine and guanine. Structure and synthesis of Uric acid and Caffeine.

Unit 6: Molecular Rearrangements and Transformations (9hrs)

Rearrangements occurring through carbocations, carbanions, carbenes and nitrenes such as Wagner-Meerwein, Demjanov, dienone-phenol, benzyl- benzilic acid, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Fries, Bayer- Villiger, Wittig, Orton, and Fries rearrangements. Peterson reaction, Woodward and Prevost hydroxylation reactions. Heck, Negishi, Sonogashira, Stille, and Suzuki coupling reactions (mechanism)

References:

1. M. B. Smith, *organic synthesis*, 3/e, academic press, 2011.
2. R. O. C. Norman and j. M. Coxon, *principles of organic synthesis*, 3/e, crc press, 1998.
3. W. Carruthers and i. Coldham, *modern methods of organic synthesis*, 4/e, cambridge University press.
4. R. R. Carey and r. J. Sundburg, *advanced organic chemistry*, part b, 5/e, springer, 2007.
5. M. B. Smith, j. March, *march's advanced organic chemistry*, 6/e, john wiley & sons, 2007.
6. J. Clayden, n. Greeves, s. Warren and p. Wothers, *organic chemistry*, 2/e, oxford University press, 2012.
7. J. J. Li, *name reactions*, 4/e, springer, 2009.
8. V. K. Ahluwalia and r. Aggarwal, *organic synthesis: special techniques*, 2/e, narosa Publishing house, 2006.
9. G. Odiyan, *principles of polymerisation*, 4/e, wiley, 2004.
10. V.r. gowriker and others, *polymer science*, wiley eastern ltd.
11. I.l. finar, *organic chemistry*, vol. Ii, 5/e, elbs, 1975.
12. J. A. Joules and k. Mills, *heterocyclic chemistry*, 4/e, oxford university press, 2004.
13. T. L. Gilchrist, *heterocyclic chemistry*, 3/e, pearson, 1997.
14. T. H. Lowry and k. S. Richardson, *mechanism and theory in organic chemistry*, 3/e Addison-wesley, 1998.

COURSE: REAGENTS &TRANSFORMATIONS IN ORGANIC CHEMISTRY

Credits: 3

Instructors: **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Understand different oxidation methods in organic chemistry	PSO I	U	C	6	0	0
2	Analyse synthetic reagents for organic transformation	PSO I	An	C	6	0	0
3	Study different reduction methods in organic chemistry	PSO I	S	C	6	0	0
4	Analyse several reactions for the formation of carbon-carbon bond	PSO II	An	C	6	0	0
5	Study the structure, synthesis and reactions of heterocyclic compounds	PSO II	S	C	8	0	0
6	Understand several molecular rearrangements and transformation	PSO I	U	C	8	0	0
7	Study the mechanism of different rearrangement reaction	PSO II	S	P	8	0	0
8	Understand the structure and synthesis of caffeine	PSO II	U	P	6	0	0

Total hours of instruction

**Course Code : **VPCH3E01

Course Title : SYNTHETIC ORGANIC CHEMISTRY (3Credits, 54h)

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH3E01 - SYNTHETIC ORGANIC CHEMISTRY (3 Credits, 54hrs)

Unit 1: Reagents for Oxidation and Reduction (9hrs)

Reagents for oxidation and reduction: Oxone, IBX, PCC, osmium tetroxide, ruthenium tetroxide, selenium dioxide, molecular oxygen (singlet and triplet), peracids, hydrogen peroxide, aluminum isopropoxide, periodic acid, lead tetraacetate. Wacker oxidation, TEMPO oxidation, Swern oxidation, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation.

Catalytic hydrogenations (heterogeneous and homogeneous), metal hydrides, Birch reduction, hydrazine and diimide reduction.

Unit 2: Organometallic and Organo-nonmetallic Reagents (9hrs)

Synthetic applications of organometallic and organo-nonmetallic reagents: Reagents based on chromium, nickel, palladium, silicon, and born, Gilman reagent, phase transfer catalysts, hydroboration reactions, synthetic applications of alkylboranes. Gilman's reagent, Tri -n-butyl tin hydride, Benzene Tricarbonyl Chromium

Unit 3: Chemistry of Carbonyl Compounds (9hrs)

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides, amides. Substitution at -carbon, aldol and related reactions, Claisen, Darzen, Dieckmann, Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Reaction with phosphorous and sulfur ylides.

Protecting groups, functional group equivalents, reversal of reactivity (Umpolung), Introduction to combinatorial chemistry.

Unit- 4. Coupling Reactions (9hrs)
Coupling Reactions: PalladiumCatalysts for C-N and C-O bond formation, Palladium catalyzed amine arylation (Mechanism and Synthetic applications). Sonogashira cross coupling reaction (Mechanism, Synthetic applications in Cyclic peptides) Stille carbonylative cross coupling reaction (Mechanism and synthetic applications). Mechanism and synthetic applications of Negishi, Hiyama, Kumada, Heck and Suzuki-Miyaura coupling reactions.

Unit 5: Multi step Synthesis (9hrs)

Multi step Synthesis**:** Synthetic analysis and planning, Target selection, Elements of a Synthesis (Reaction methods, reagents, catalysts, solvents, protective groups for hydroxyl, amino, Carbonyl and carboxylic acids, activating groups, leaving groups synthesis and synthetic equivalents. Types of selectivities (Chemo, regio, stereo selectivities) synthetic planning illustrated by simple molecules, disconnections and functional group interconversions, uplong reactions and use in synthesis, Introduction to retrosynthetic analysis, Synthesis of longifolene, Corey lactone, Djerassi Prelog lactone

Unit 6: Phase transfer catalysis and Crown ethers (9hr)

Phase transfer catalysis: Introduction, definition, mechanism of phase transfer catalysis, advantages and types of phase transfer catalysts. Preparation of catalysts and applications: substitution, condensation, oxidation and reduction reactions.

Crown ethers: Introduction, nomenclature, features, nature of donor site. General synthesis of Crown ethers. Synthetic applications-alkylation, anhydride formation, generation of carbenes, aromatic substitution and displacement reactions

References:

1. M. B. Smith, *organic synthesis*, 3/e, academic press, 2011.
2. S. Warren and p. Wyatt, *organic synthesis: strategy and control*, john wiley
3. S. Warren: *organic synthesis: the disconnection approach*, john wiley
4. H. O. House: *modern synthetic reactions*, w. A. Benjamin
5. W. Carruthers and i. Coldham, *modern methods of organic synthesis*, 4/e, cambridge University press.
6. T. W. Greene and p. G. M. Wuts: *protecting groups in organic synthesis*, 2nd ed., john wiley
7. M b smith and j. March: *advanced organic chemistry-reactions, mechanisms and structure,* 6th ed., john wiley
8. T. H. Lowry and k. S. Richardson: *mechanism and theory in organic chemistry*, 3rd ed.
9. R. R. Carey and r. J. Sundburg, *advanced organic chemistry*, part a and b, 5/e, springer, 2007
10. A. Pross: *theoretical and physical principles of organic chemistry*, john wiley
11. T.w. graham solomons: *fundamentals of organic chemistry*, 5th ed., john wiley
12. I. L. Finar: *organic chemistry* volumes 1 (6th ed.), pearson
13. J. Clayden, n. Green, s. Warren and p. Wothers: *organic chemistry*, 2/e, oxford university Press
14. J. J. Li, *name reactions*, 4/e, springer, 2009.
15. N. K. Terret: *combinatorial chemistry*, oxford university press, 1998.

COURSE: SYNTHETIC ORGANIC CHEMISTRY

Credit :3

Instructors: **Total hours: 54**

3hrs/week

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Understand the reagents for oxidation and reduction	PSO I	U	C	6	0	0
2	Analyse homogeneous and heterogeneous catalytic hydrogenation	PSO I	An	C	8	0	0
3	Evaluvate synthetic applications of organometallic and organo-nonmetallic reagents	PSO II	E	C	6	0	0
4	Understand the chemistry and reactivity of carbonyl compounds	PSO I	U	F	6	0	0
5	Study the mechanism and synthetic applications of coupling reactions	PSO II	S	P	6	0	0
6	Evaluate the methods involved in multistep synthesis	PSO II	E	P	8	0	0
7	Analyse aspects of retrosynthetic analysis	PSO II	An	P	8	0	0
8	Understand the concepts of phase transfer catalysis	PSO I	U	C	6	0	0

Total hours of instruction

Department : Chemistry

Programme : M.Sc Chemistry

Semester : IV

Course Code : VCH4C13

Course Title : : ADVANCED TOPICS IN CHEMISTRY
Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH4C13- ADVANCED TOPICS IN CHEMISTRY (4Credits, 72hrs)

Unit 1: Chemistry of Nanomaterials (9hrs)
History of nanomaterials- Classification.Size- dependence of properties. Electronic structure theory of metals and semiconductors. Quantum size effects.
Synthesis of nanostructures: bottom-up-approach, top- down approach, self-assembly, lithography, molecular synthesis, template assisted synthesis.

Methods of characterization: Electron microscopies-SEM,TEM. Scaning prob microscopies- STM, AFM. X-ray photoelectron spectroscopy(XPS), Dynamic light scattering(DLS), X-ray diffraction(XRD).

Applications: Nanoelectronics, nanosensors, nanocatalysts, nanofilteration, diagnostic and therapeutic applications and targeted drug delivery.
Introduction to graphenes and fullerenes.

Unit 2: Green Chemistry (9hrs)
Introduction, the need of green chemistry, principles of green chemistry, planning of green synthesis, tools of green chemistry. Green reactions- Aldol condensation, Cannizaro reaction and Grignard reaction.Comparison of the above green reactions with classical reactions.Green preparations. Applications of phase transfer catalysis. Introduction to microwave organic synthesis, Applications: environmental, solvents, time and energy benefits.

Unit 3: Introduction to Computational Quantum Chemistry (9hrs)
Electronic structure of molecules-Review of Hartee-Fock SCF method. Basis sets STO_s and GTO_s . Nomenclature of Basis sets. Semi empirical and ab initio methods. Calculations using Gaussian programme . Spesification of molecular geometry using a) Cartisian coordinates and b) Internal coordinates. The Z-matrix . Z- matrices of some simple molecules like H_2,H_2o,

formaldehyde ammonia and methanol.

Unit 4: Supramolecular Chemistry (9hrs)

Concepts and language. Molecular recognition: Molecular receptors for different types of molecules, design and synthesis of coreceptors and multiple recognition. Strong, weak and very weak Hydrogen bonds.Utilisation of H-bonds to create supramolecular structures. Use of H-bonds in crystal engineering and molecular recognition.

Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices Some examples of self- assembly in supramolecular chemistry.

Unit 5: Medicinal Chemistry (9hrs)

Drug Design and Relationship of Functional Groups to Pharmacologic Activity: Introduction, different classes of drugs, drug action, pro drugs, physico chemical properties of drugs and their pharmacologic activity , SAR and QSAR , factors governing ability of drugs. Drug design, factors governing drug design, rational approach to drug design, general methods of drug synthesis.Analgesics(Phenazones and phenyl butazones as examples), antipyretic(paracetamol), antibiotics, pencillins, chloramphanicol.

Unit 6: Combinatorial Chemistry (9hrs)

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, requirements-resins, Linkers. Reactants for solid phase synthesis. Methods of Parallel synthesis: Haughton`s tea bag procedure. Automated parallel synthesis. Methods in mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis. Structure determination of active compounds- Deconvolution. Methods in deconvolution-recursive deconvolution, tagging use of decoded sheets. Planning and designing of combinatorial synthesis. Spider like scaffolds, drug molecules. Limitations of combinatorial chemistry.

Unit 7: Introduction to Industrial Catalysis (9hrs)

Structure and chemical nature of surfaces. Physisorption and chemisorptions. Energy exchange at surface. Determination of surface area and pore structure of catalysts - physical adsorption methods, X-ray methods, mercury intrusion method, chemisorptions methods. Determination of surface acidity-TPD method. Catalyst selectivity, effect of pore size on selectivity. Homogeneous and heterogeneous catalysts. Preparative methods for heterogeneous catalysts- precipitation and co-precipitaion methods, sol gel method, flame hydrolysis. Preparation of Zeolites and silica supports. Mesoporous materials. Introduction to Phase transfer catalysis, biocatalysis, nanocatalysis and polymer supported catalysis. Application of heterogeneous catalysts in water gas shift reaction, ammonia synthesis, catalytic cracking, Fisher-Tropsch process, threeway catalysis.

Unit 8: Renewable Energy Sources (9hrs)

World's reserve of commercial energy sources and their availability, various forms of energy, Renewable and conventional energy systems, comparison - coal, oil and natural gas, availability, applications, merits and demerits. Renewable energy sources - solar energy, nature of solar radiation, components- solar heaters, solar cookers, water desalination. Photovoltaic generation – basics, merits and demerits of solar energy. i) Solid state junction solar cells:- principle of solar cells, Fabrication of CdS/Cu_2S and $CdS/CuInSe_2$ solar cells, performance testing, stability and efficiency consideration. Dye sensitized solar cells (DSSC)-Working principle, Fabrication of DSSCs based on TiO_2 and ZnO, stability and performance of dyes.

References:

1. C.P.Poole(Jr.) and F.J. Owens, Introduction to Nanotechnology,Wiley India, 2007.
2. G.A.Ozin and A.C.Arsenault, Nanochemistry, RSC Publishing,2008.
3. T.Pradeep, The essentials of Nanotechnology, Tata McGra Hill, New Delhi, 2007.
4. K.J.Klabunde(Ed.), Nanoscale Materials in Chemistry, John Wiley&Sons, 2001.
5. P.T.Anastas and J.C.Warner, Green Chemistry:Theory and Practice, Oxford University Press, 1998.

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7.J.H.Clark,The Chemistry of waste minimization, Blackie Academic, London,1995.

8.C.J.Cramer, Essentials of computational Chemistry:Theories and models, John Wiley & Sons,2002.

9.Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons,1999.

10.Errol G Lewars Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, Springer,2001.

11.David Young, Computational Chemistry, Wiley –Interscience, 2001.

12.F. Vogtle, Supramolecular Chemistry, John Wiley & Sons, Chichester, 1991.

13.J.M.Lehn, Supramolecular Chemistry, VCH.

14.Lemke, Williams, Roche and Zito, Principles of Medicinal Chemistry, 7/e, Wolters Kluwer, 2012.

15.G.Thomas, Fundamentals of Medicinal Chemistry, Wiley.

16. G.Gringauz, *Introduction to Medical Chemistry,* Wiley-VCH, 1997.
17. Harkishan Singh and V.K.Kapoor, *Medicinal and Pharmaceutical Chemistry,* Vallabh Prakashan, 2008.
18. W.Bannwarth and B.Hinzen, *Combinatorial Chemistry-From Theory to Application, 2nd*

Edition, Wiley-VCH, 2006.
19. A.W.Czarnik and S.H.DeWitt, *A Practical Guide to Combinatorial Chemistry*, 1st Edition, American Chemical Society, 1997.
20. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, 6 Edn., Wiley, 2011.
21. Jens Hajen, *Industrial Catalysis: A Practical Approach.* 2nd Edn., Wiley VCH, 2006.
22. Dipak Kumar Chakrabarty, *Adsorption and Catalysis by Solids*, New Age. 2007.
23. C.H. Bartholomew and R.J. Farrauto, *Fundamentals of Industrial Catalysis Process,* 2nd Edn. Wiley & Sons Inc. 2006.
24. Woodruff, D. P. and Delchar T. A., *Modern Techniques of Surface Science*, Cambridge Solid State Science Series, 1994.
25. Kurt K. Kolasinski, *Surface Science: Foundations of Catalysis and Nanoscience,* 3rd Edn., Wiley U. K., 2012.
26. Bansal N K, Kleeman M and Mells M, *Renewable Energy Sources and Conversion Technology*, Tata McGraw-Hill. (1990)
27. Kothari D.P., *"Renewable energy resources and emerging technologies",* Prentice Hall of India Pvt. Ltd., 2008.
28. Rai G.D, *"Non-Conventional energy Sources"*, Khanna Publishers, 2000

Course Outcomes:

COURSE: ADVANCED TOPICS IN CHEMISTRY **Credits: 4**

Instructors: Susan Samuel ,Anjali T R **Total hours: 72, 4hrs/week**

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Acquire proficiency in nanochemistry and nanomaterials	PSO III	An	F	9	0	
2	Study of green chemistry to help reduce the damage of environment caused by man-made materials	PSO III	Ap	C	9	0	0
3	Explain the calculations using Gaussien programme	PSO II	E	P	7	0	2
4	Implement concepts and language of supramolecular chemistry	PSO III	An	C	9	0	0
5	Understand the drug design and relationship of functional group to pharmacologic activity	PSO III	U	F	9	0	0
6	Explain the tools of combinatorial chemistry.	PSO III	An	P	9	0	0
7	Use TPD method for determination of surface acidity	PSO I	E	F	9	0	0
8	Describe renewable and conventional energy resources	PSO I	U	F	9	0	0
	Total hours of instruction				70		2

Course Code : VCH4E22

Course Title : INDUSTRIAL CATALYSIS (ELECTIVE)
Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH4EO5 - INDUSTRIAL CATALYSIS (ELECTIVE) (4 Credits, 72hrs)

Unit 1: Introduction to Adsorption process (9hrs)
Intermolecular interactions, physisorption – the forces of adsorption – dispersion and repulsive forces – classical electrostatic interactions – adsorbate-adsorbate interactions, chemisorption, potential energy curves, thermodynamics of adsorption – isothermal and adiabatic heats of adsorption – variation of heats of adsorption with coverage, adsorption isotherms, Langmuir, BET and Freundlich, kinetics of chemisorption – activated and non-activated chemisorption – absolute rate theory – electronic theories, hysteresis and shapes of capillaries.

Unit 2: catalytic preparative methods (9hrs)
General preparative methods-precipitation and co-precipitation- sol gel process- flame hydrolysis-supported catalysts from CVD and related techniques – dispersed metal catalysis.
Catalyst manufacture-equipment-scope and goals-catalyst prepared by precipitation-solution and slurry transfer-filtration-drying-containers, trays and other drying auxillaries; calcining;rewashing and ion exchange;pulverization;pilling and extrusion; crushing and screening to produce granules; coating(not impregnation); impregnation to orient the coating material to support- anchor coating or wash coating.

Unit 3: Catalyst - Praparative Methods(9hrs)
Surface area and porosity measurement – measurement of acidity of surfaces; Support materials – preparation and structure of supports – surface properties, preparation of catalysts – of some selected zeolites – zeolites A, X and Y, pentasils – ZSM-5, ZSM-11, shape selective catalysis by zeolites.

Unit 4: Deactivation of Catalysts (9hrs)
Deactivation of catalysts, classification of catalyst deactivation processes, poisoning of catalysts, coke formation on catalysts, metal deposition on catalysts, sintering of catalysts, Regeneration of deactivated catalysts, feasibility of regeneration, description of coke deposit and kinetics of regeneration.

UNIT 5: Phase Transfer Catalysis (9hrs)

Basic concepts in phase transfer catalysis – phase transfer catalyzed reactions – basic steps of phase transfer catalysis – effect of reaction variables on transfer and intrinsic rates – outline of compounds used as phase transfer catalysts. Use of quaternary salts – macrocyclic and macrobicyclic ligands – PEG's and related compounds –use of dual phase transfer catalyst or co-catalyst in phase transfer systems –separation and recovery of phase transfer catalysts. Insoluble phase transfer catalysts.

UNIT 6: Biocatalysis (9hrs)

Enzymes – an introduction to enzymes – enzymes as proteins – classification and nomenclature of enzymes – structure of enzymes – how enzymes work – effect on reaction rate – thermodynamic definitions – catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis – specific catalytic groups contributing to catalysis. Immobilized biocatalysts – definition and classification of immobilized biocatalysts – immobilization of coenzymes.

UNIT 7: Industrial Catalysis-1 (9hrs)

Oil based chemistry; catalytic reforming; catalytic cracking; paraffin cracking; naphthenic cracking; aromatic hydrocarbon cracking; isomerization; hydrotreatment; hydrodesulphurization; hydrocracking; steam cracking; hydrocarbons from synthesis gas; Fisher-Tropsch process, Mobil process for conversion of methanol to gasoline hydrocarbons. Catalysis for environmental protection, removal of pollutants from exhausts, mobile and static sources.

UNIT 8: Industrial Catalysis-II (9hrs)

Hydroformylation of olefins, carbonylation of organic substrates, conversion of methanol to acetic acid, synthesis of vinyl acetate and acetic anhydride, palladium catalyzed oxidation of ethylene, acrylonitrile synthesis, Zeigler-Natta catalysts for olefin polymerization. Propene polymerization with silica supported metallocene/MAO catalysts.

References:

1. A. Clark, *"Theory of adsorption and catalysis",* Academic Press, 1970.
2. J.M. Thomas & W.J. Thomas, *"Introduction to principles of heterogeneous catalysis",*
3. Academic Press, New York, 1967.
4. R.H.P. Gasser, *"An introduction to chemisorption and catalysis by metals",* Oxford, 1985.
5. D.K Chakraborthy, *"Adsorption and catalysis by solids",* Wiley Eastern Ltd. 1990.
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8. R. Szostak, *"Molecular sieves: principles of synthesis and identification*", Van Nostrand, NY,1989.

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13. R.J. Farrauto and C.H. Bartholomew, *"Fundamentals of Industrial Catalytic Processes",*
14. Blackie Academic and Professional – Chapman and Hall, 1997.
15. R. Pearce and W.R. Patterson, *"Catalysis and chemical processes*", Academic press, Leonard Hill, London, 1981.

Course outcome:

COURSE: INDUSTRIAL CATALYSIS **Credits: 4**

Instructors: Susan Samuel ,Anjali T R **Total hours: 72, 4hrs/week**

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Compare physisorption and chemisorptions	PSO I	U	P	9	0	0
2	Analyse kinetics of heterogeneous catalysis.	PSO I	E	C	9	0	0
3	Explain Langmuir, BET and Freundlich isotherms	PSO II	U	P	7	0	2
4	Describe the different methods for the preparation and deactivation of catalysts.	PSO I	An	P	9	0	0
5	Understand the basic principles of phase transfer catalysed reactions.	PSO I	U	F	9	0	0
6	Discuss the biocatalysts and their immobilization.	PSO I	U	F	9	0	0
7	Built knowledge on the catalysts used for environmental protection	PSO III	E	F	9	0	0
8	Describe the role of heterogeneous catalysts	PSO I	U	F	9	0	0
	Total hours of instruction				70		2

Course Code : VCH4C13

Course Title : INSTRUMENTAL METHODS OF ANALYSIS

Learning Objectives (If already given in the syllabus) :

Syllabus (Unit-wise) with Hours :

VPCH4C12 INSTRUMENTAL METHODS OF ANALYSIS (4 Credits, 72 hrs)

Unit 1: **Errors in Chemical Analysis (9hrs)**

Treatment of analytical data, accuracy and precision, Absolute and relative errors, classification and minimization of errors, significant figures, Statistical treatment- mean and standard deviation, variance, confidence limits, student-t and f tests, detection of gross errors, rejection of a result-Q test. Least square method, linear regression; covariance and correlation coefficient

Unit 2: **Conventional Analytical Procedures (9hrs)**

Gravimetry: **s**olubility product and properties of precipitates-nucleation, growth and aging, co-precipitation and post precipitation, drying and ignition. Inorganic precipitating agents: NH_3, H_2S, H_2SO_4, $(NH_4)_2MoO_4$ and NH_4SCN.

Organic precipitating agents: oxine, cupron, cupferron, 1-nitroso-lnaphthol, dithiocarbamates, Acid-Base and precipitation titrations: theory of neutralisation titrations, indicators for acid/base titrations, titration curves of strong acid, strong base, weak acid, weak base and polyprotic acids. Buffer solutions.

Titrations in nonaqueous media. Different solvents and their selection for a titration. Indicators for non-aqueous titrations

Redox titrations: Permanganometry, dichcrometry, iodometry, cerimetry. Variation of potential during a redox titration, formal potential during a redox titration, Redox indicators.

Precipitation titrations, adsorption indicators

Complexometric titrations: Types of EDTA titrations (direct, back, replacement, alkalimetric and exchange reactions), masking and demasking agents, selective demasking, metal ion indicators - murexide, eriochrome black T, Patton and Reeder's indicators, bromopyrogallol red, xylenol orange, variamine blue.

Unit 3: Electro Analytical Methods- I (9hrs)

Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements. Principles and instrumentations of polarograohy Applications of polarography, Amperometry;biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry.

Unit 4 Analysis of Biomolecules II (9hrs)

Introduction, single molecule detection and characterization, mass spectrometry in structural biology, Voltametry in in-vivo chemical analysis of nervous system. Enzyme and immuno techniques- Enzyme based assay. ELISA, RIA, Fluorescent techniques, Western blotting, Biosensors, and chemosensors. Nano techniques - Detection using fluorescence. DNA sequencing, sequencing of proteins*.

Unit 5 Optical Methods - I (9 hrs)

Fundamental laws of spectrophotometry, nephelometry and turbidometry and fluorimetry. UV-visible and IR spectrophotometry – instrumentation, single and double beam instruments, Spectrophotometric titrations. Atomic emission spectrometry – excitation sources (flame, AC and DC arc), spark, inductively coupled plasma, glue discharge, laser microprobes, flame structure, instrumentation, and qualitative and quantitative analysis. Atomic absorption spectrometry: sample atomization techniques, instrumentation, interferences, background correction, and analytical applications.

Unit 6 Optical Methods - II (9 hrs)

Theory, instrumentation and applications of: - Atomic fluorescence spectrometry, X-ray methods,: X-ray absorption and X-ray diffraction, photoelectron spectroscopy, Auger, ESCA. SEM, TEM, AFM

Unit 7: **Thermal and Radiochemical Methods (9hrs)**

Thermogravimetry(TG), Differential Thermal Analysis(DTA) and Differential Scanning Calorimetry(DSC) and their instrumentation. Thermometric Titrations.

Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications.Principle and applications of isotope dilution methods.

Unit 8: Chromatography (9 hrs)

Chromatography-classification-column-paper and thin layer chromatography. HPLC-outline study of instrument modules. Ion – exchange chromatography-Theory. Important applications of chromatographic techniques. Gel Permeation Chromatography.

Gas chromatography – basic instrumental set up-carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Qualitative and quantitative studies using GC, Preparation of GC columns, selection of stationary phases of GLC, Gas adsorption chromatography, applications, CHN analysis by GC

References:

1. J.M. Mermet, M. Otto, R. Kellner, *Analytical Chemistry*, Wiley-VCH, 2004.

2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, *Fundamentals of Analytical Chemistry*, 9th Edn., Cengage Learning., 2014.

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5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, *Vogel's Text Book of Quantitative Chemical Analysis*, 5th Edn., John Wiley& sons,1989.

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12. V.K. Ahluwalia, *Green Chemistry: Environmentally Benign Reactions*, CRC, 2008.

13. F.W. Fifield, D. Kealey, *Principles and Practice of Analytical Chemistry*, Blackwell Science, 2000

Course outcome:

COURSE: INSTRUMENTAL METHODS OF ANALYSIS **Credits: 4**

Instructors: Susan Samuel ,Anjali T R **Total hours: 72, 4hrs/week**

	Course outcome	POs/ PSOs	CL	KC	CLASS SESSIONS (app.)	Tutorial (if any) (Hrs)	Lab(Hrs)
1	Acquire proficiency in statistical analysis and error estimation	PSO I	U	P	7	0	2
2	Analyses how health, disease and modern medicine are all rooted in biological chemistry	PSO III	Ap	C	9	0	0
3	Explain the principles of gravimetric inorganic precipitating agent like NH_3,H_2S,$(NH_4)_2MoO_2$ AND NH_4SCN	PSO I	U	F	9	0	0
4	Describe neutron activation analysis with quantitative analysis	PSO II	Ap	P	2	0	0
5	Understand the capabilities and limitations of optical instrumental methods	PSO I	U	F	9	0	0
6	Explain the instrumental component and principals of operation	PSO I	U	F	9	0	0
7	Built knowledge on chromatographic method, detectors and CHN analysis by GC	PSO II	E	F	9	0	0
8	Describe TGA,DTA,DSE and their instrumentation	PSO I	U	F	7	0	0
9	Describe amperometry,coulometry, chronopotentiometry,	PSO I	U	F	9	0	0

	anodic stripping voltametry						
	Total hours of instruction				70		2