UNIVERSITY OF CALICUT

(Abstract)

M.Sc programme in Chemistry under Credit Semester System (PG) -in affiliated colleges-Modified Syllabus-approved– implemented-with effect from 2010 admissions-Orders issued.

GENERAL & ACADEMIC BRANCH-IV 'J' SECTION

No. GA IV/J2/4684/10 Calicut University PO, Dated 17.02.2012

Read: 1. U.O.No. GAIV/J1/1373/08 dated 23.07.2010.
2. U.O. No. GAIV/J2/4684/08 dated 30.07.2010.
3. U.O.No. GAIV/J2/4684/10 dated 19.01.2011
4. Minutes of the meeting of the Board of Studies in Chemistry held on 19.11.2011.
5. Orders of the Registrar on 08.02.2012
6. Orders of the Vice Chancellor on 14.02.2 012 in the file of even no.

O R D E R

As per University Order read as first, Credit Semester System was implemented to all PG programmes in affiliated Arts and Science Colleges and Self Financing Centers of the University with effect from 2010 admission onwards.

The scheme and syllabus for the 1st semester of M.Sc Programme in Chemistry under CSS PG was implemented vide paper read as second above. Vide paper read as third above, the syllabus of M.Sc. Chemistry programme under CSS PG for the II, III, & IV semesters was implemented.

The Board of Studies in Chemistry (PG) in its meeting held on 19.11.2011 approved the modified syllabus of M.Sc. Chemistry programme under CSS PG with effect from 2010 admission vide paper read as third.

The Vice-Chancellor, considering the exigency, exercising the powers of the Academic Council has approved the item no. 01 of the minutes, subject to ratification by the Academic Council.

Sanction has therefore been accorded for implementing the modified Syllabus of M.Sc programme in Chemistry under CSS PG 2010 with effect from 2010 admission.

Orders are issued accordingly. Scheme and Syllabus appended.

Sd/-
ASSISTANT REGISTRAR (G & A-IV)
For REGISTRAR

Forwarded/By Order

Sd/-
SECTION OFFICER

To

The Principals of affiliated Colleges offering MSc programme in Chemistry

Copy to:

PS to VC,PA to Registrar,Chairman,B/S Chemistry PG,CE,EX,DRIII,DR,PG,EGI,Enquiry,System Administrator (with a request to upload in the University website),Information Centres,GAI`F``G`, GAII,III/SF/FC/DF

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN)

Regulations and Syllabus
with effect from 2010 admission

Preamble

The Board of Studies in Chemistry (PG) at its meeting held on 21.06.2010 considered the introduction of Credit Semester System (CSS) in affiliated colleges for the PG programmes in Chemistry and resolved to implement the CSS pattern from 2010 admission onwards. The revised programme pattern; syllabus, distribution of credits and scheme of evaluation, etc. approved by the Board are given below:

Pattern of the Programme

(a) The name of the programme shall be M.Sc. Chemistry under CSS pattern.

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

(c) Eligibility for admission will be as per the rules laid down by the University from time to time.

(d) Details of the programme offered for the programme are given in Table I. 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 practicals and 1 hour for seminar.

Theory Courses

In each semester there will be three theory courses. All the theory courses in the first and second semesters are core papers. In the third semester there will be two core theory courses and one elective course. Colleges can choose any one of the elective courses given in table 1. In the fourth semester there will be one core courses and two elective courses. College can choose any two elective courses from those given in table 1. However a candidate may be permitted to choose any other elective courses without giving any lecture classes.

Practicals: In each semester there will be three core practical courses (2 credits each). However practical examination will be conducted only at the end of the second semester for CHPO1, CHPO2, CHPO3 and at the end of fourth semester for CHPO4, CHPO5, CHPO6.

Project and Viva Voce: Each student will have to do an independent research project work during the programme under the guidance of a faculty member of the college/ scientists of recognized research institutions and to submit the dissertation at the end of the fourth semester for evaluation (5 credits). There will be a comprehensive viva voce (3 credits) at the end of

the fourth semester. The viva voce will be based on the theory and practical courses and the project work.

Dr. K. Krishnankutty
Chairman
BOS in Chemistry (PG)

TABLE I

Courses offered for M.Sc. Chemistry Programme under CCSS in Affiliated Colleges

	Course Code	Course Title	Instruction/ Week	Credits
SEMESTER I	CH1CO1	Theoretical Chemistry I	4	4
	CH1CO2	Inorganic Chemistry I	4	4
	CH1CO3	Organic Chemistry I	4	4
	CH1PO1	Inorganic Chemistry Practical I	4	
	CH1PO2	Organic Chemistry Practical I	4	
	CH1PO3	Physical Chemistry Practical I	4	
		Total Credits (Core)		12
SEMESTER II	CH2CO4	Theoretical Chemistry II	4	4
	CH2CO5	Physical Chemistry I	4	4
	CH2CO6	Organic Chemistry II	4	4
	CH2PO1	Inorganic Practical I	4	4
	CH2PO2	Organic Practical I	4	4
	CH2PO3	Physical Practical I	4	4
		Total Credits (Core)		24
SEMESTER III	CH3CO7	Physical Chemistry II	4	4
	CH3CO8	Inorganic Chemistry II	4	4
	CH3PO4	Inorganic Practicals II	4	
	CH3PO5	Organic Practicals II	4	
	CH3PO6	Physical Practicals II	4	
	CH3EO1	Synthetic Organic Chemistry	4	4
	CH3EO2	Natural Products	4	4
	CH3EO3	Polymer Chemistry	4	4
		Total Credits – Core Elective		8 4

SEMESTER IV	CH4CO9	Advanced Topics in Chemistry	4	4
	CH4PO4	Inorganic Chemistry Practical II	4	4
	CH4PO5	Organic Chemistry Practical II	4	4
	CH4PO6	Physical Chemistry Practical II	4	4
	CH4EO4	Instrumental Methods of Analysis	4	4
	CH4EO5	Computational Chemistry	4	4
	CH4EO6	Material Science	4	4
	CH4EO7	Industrial Catalysis	4	4
	CH4EO8	Bioinorganic and Organometallic Chemistry	4	4
	CH4PrO1	Research Project and Viva Voce		5+3=8
		Total Credits - Core Elective Project		16 8 8
		TOTAL CREDITS OF THE PROGRAMME		
		CORE		60
		ELECTIVE		12
		PROJECT AND VIVA VOCE		8
Total Credits				**80**

UNIVERSITY OF CALICUT
M.Sc. CHEMISTRY CSS PATTERN – SEMESTER I

CH1CO1 – THEORETICAL CHEMISTRY – I (4 Credits) (72 h)

UNIT I : The Foundations of Quantum Mechanics (9 h) . Historical background of quantum mechanics. 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.

UNIT II : Quantum mechanics of translational & vibrational motions (9 h). Particle in a one-dimensional box with infinite potential walls, important features of the problem; Free particle in one-dimension; Particle in a one-dimensional box with finite potential walls (or particle in a rectangular well) – tunneling; Particle in a three dimensional box, separation of variables, degeneracy.

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 III : Quantum mechanics of Rotational motion (9 h) . Co-ordinate systems:- Cartesian, cylindrical polar and spherical polar coordinates and their relationships. Rigid rotator (complete treatment): The wave equation in spherical polar coordinates, planar rigid rotor (or particle on a ring), the Phi-equation, solution of the Phi-equation, handling of imaginary wave functions, wave functions in the real form; Non-planar rigid rotor (or particle on a sphere), 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), polar diagrams of spherical harmonics.

Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x, L_y, L_z,), commutation relations between these operators, spherical harmonics as eigen functions of angular momentum operators L_x & L_z, Ladder operator method for angular momentum, space quantization.

UNIT IV : Quantum Mechanics of Hydrogen-like Atoms (9h). 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 V : Approximation methods in quantum mechanics (9 h). 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 $e^{-\alpha r^2}$ 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 VI : Quantum mechanics of many-electron atoms (9 h). 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).

UNIT VII : Chemical bonding in diatomic molecule (9 h). 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 VIII : Chemical Bonding in polyatomic molecules (9 h). 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.

References

1. F.L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill, 1968.
2. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc., 2009.
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.

UNIVERSITY OF CALICUT
M.Sc. CHEMISTRY CSS SYSTEM – SEMESTER I

CH1CO2 – INORGANIC CHEMISTRY – I - 4 CREDIT (72 h)

UNIT I : (9 h). Acid base theories – strength of acids and bases, Factors governing acid strength, solvent leveling, effect of hard and soft acids and bases, super acids, chemistry of non aqueous solvents – liquid NH_3, SO_2, H_2SO_4 and HF. Heterogeneous acid-base reactions – surface acidity, Solid and molten acids in industrial processes.

UNIT II (9 h). Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, Boron cluster compounds, Wade's rule, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions, Carboranes, Metalloboranes, Borazine s and Borides.

UNIT III (9 h). Phosphorus-nitrogen compounds; Phosphazene, cyclo- and linear phosphazenes. Phosphorus-sulphur compounds; Sulphur-nitrogen ring and chain compounds – synthesis, structure, bonding and uses. Silicones – Synthesis, structure and applications. Carbides and silicides. Silicates and alumino silicates – framework of silicates, structure and application,

UNIT IV (9 h). Standard reduction potentials and their diagrammatic representations Ellingham diagram. Latimer and Frost diagram. Pourbaux diagrams. Metallic corrosion and passivity, Isopoly and heteropoly anions of early transition metals.

UNIT V (9 h). Errors and treatment of analytical data, limitations of analytical methods, accuracy and precision, classification and minimization of errors, significant figures, standard deviation, statistical treatment of data, students tests, confidence limit, Q test, Method of least squares.

UNIT VI (9 h). Theory Indicators, Acid-base, redox, absorption, complexometric and luminescent indica tors, Titrations in non-aqueous solvents, Complex formation titrations, Principles of gravimetric analysis, Formation and properties of precipitates, Co-precipitation, Precipitation from homogeneous solution, Washing of the precipitate, ignition of the precipitate, Fractional precipitation, Organic precipitants.

UNIT VII (9 h). Introduction to co-ordination Chemistry – Stereochemistry of coordination compounds. Formation constants, factors influencing stability, methods of determination of stability consta nts, stabilization of unusual oxidation states. Chelate-macrocyclic and template effects, ambidentate and macrocyclic ligands. Valence bond theory and its limitations.

UNIT VIII (9 h). The crystal field and ligand field theories, orbital splitting in octahedral, tetrahedral and square planar fields. Factors affecting crystal field splitting, spectrochemical and nephelauxetic series, Racah parameters, Jahn-Teller effect, MO theory – composition of ligand

group orbitals. MO diagram of complexes with and wi thout pi-bonding. The f-orbitals and f-block complexes.

References

1. D.F. Shriver, P.W. Atkins and C.H. Langford, *Inorganic Chemistry*, ELBS, 1990.
2. J.E. Huheey, e.A. Keiter and R.L. Keiter, *Inorganic Chemistry, Principles, Structure and Reactivity*, Pearson Education, 1990.
3. F.A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, 5th Edition, John Wiley and Sons, 1988.
4. B. Douglous, D.H. McDanials and J.J. Alexander, *Concepts and Models in Inorganic Chemistry*, Oxford and IBH Publishing Co. Pvt. Ltd., 1965.
5. L.V. Azaroff, *Introduction to Solids*, McGraw Hill, NY, 1960.
6. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denny, *Vogel's Text book of Quantitative Chemicals Analysis*, 5th Edition, ELBS, 1989.
7. Skoog, West and Holler, *Fundamentals of Analytical Chenustry,* 8th Edition, Thomson and Brooks, 2004.
8. C.E. Houecroft, *Cluster molecules of p-block elements*. Oxford Scientific Publications, 1994.
9. D. Sutton, *Electronic Spectra of Transition Metal Complexes*, McGraw Hill, 1968.
10. J.C. Blair, Jr. (Ed.), *The Chemistry of Coordination Compounds*, Reinhold Pub. Cor., 1960.
11. L.F. Lindoy, *The Chemistry of Macrocyclic Ligands and Complexes*, Cambridge University Press, 1989.
12. J.D. Lee, *Concise Inorganic Chemistry*, 5th Edition, Oxford University Press, 2008.
13. Wahid U Malik, G.D. Tuli, R.D. Madan, Selected Topics in Inorganic Chemistry, S. Chand and Company Reprint 2009.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER I

CH1CO3 – ORGANIC CHEMISTRY – I (4 Credits) (72 h)

UNIT I : (9 h). Delocalized chemical bonding, Electron Delocalization, Resonance and Aromaticity: Qualitative application of Huckel MO theory and perturbation theory to systems containing delocalized electrons. Delocalized electrons and Resonance, Resonance hybrid an d resonance energy. Criteria for Aromaticity and Antiaromaticity, MO description of Aromaticity and Antiaromaticity. Homoaromaticity, Mobius twist and Aromaticity. Aromaticity of Annuelens and heteroannulenes, Fullerines, and fused ring systems. Stability of benzylic cations and radicals. Effect of delocalized electrons on pKa.

Hydrogen bonding: Inter- and intramlecular hydrogen bonding. Range of the energy of hydrogen bonding. Effect of hydrogen bond on conformation, physical and chemical properties of o rganic compounds, vilatility, acidity, basicity and stability of hydrates of carbonyl compounds. Stabilization of hydrates of glyoxal and chloral, and ninhydrin. High acid strength of maleic acid compared to fumaric acid.

UNIT II : (9 h). Basic concepts in the study of organic reaction mechanisms: Application of Experimental criteria to mechanistic studies, Thermodynamic and kinetic data, Curtius-Hammet principles, Kinetic versus thermodynamic control. Acidity constant, Hammet acidity function. Reactive intermediates and their characterizatin. Isotope effect (labeling experiments), Stereochemical correlations.

Neighbouring group participation, participation of carboxylate ion, halogen, hydroxyl group, acetoxy group, phenyl group and pi -bond.

Structure and reactivity, 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 SN1-SN2 reactions. 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.

References: (Unit I and II)

1. J. March, *Advanced Organic Chemistry*, 4th Edition, John Wiley and Sons, 1992.
2. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, Harper Collins, 1987.
3. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry* (Parts A & B), 3rd Edition, Plenum Press, 1990.
4. R.A.Y. Jones, *Physical and Mechanistic Organic Chemistry*, Cambridge University Press, 1979.

UNIT III : Isomerism-I (9 h): 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 notations in cyclic and acyclic compounds.

Optical isomerism of compounds containing one or more asymmetric carbon atoms, Enantiotopic, Homotopic, Diastereotopic hydrogen atoms, Prochiral centre.

Optical isomerism in Biphenyls, Allenes and Nitrogen and Sul phur compounds, Conditions for optical activity, R and S notations.

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. Methods of determination of the configuration of geometrical isomers in acyclic acid cyclic systems, inter conversion of geometrical isomers.

Stereochemistry of Aldoximes and ketomines – Naming – isomerism – methods of determining configurations.

UNIT IV : Isomerism-II (9 h): Asymmetric Synthesis: The chiral pool: Alpha amino acids 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 sulfoxides in controlling the reduction of ketones, Camphor derivative in Diels Alder reaction and radical reactions.

Chiral reagents: BINOL, tartrates, lithium di(1-phenyl ethyl) amide.

Chiral catalysts: Rhodium and ruthenium catalysts with chiral phosphine ligands like (R)BINAP, (R,R)DIOP. Enzymatic methods.

References

1. J. March, *Advanced Organic Chemistry*, 4th Edition, John Wiley and Sons, 1992.
2. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edition, New Age International.
3. Kalsi, *Stereochemistry of Organic Compounds*, Wiley Eastern.
4. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
5. E. Eliel and S.H. Wilen, *Stereochemistry of Organic Compounds*, John Wiley, 1994.

UNIT V : Conformational Analysis – I (9 h): Difference between configuration and confirmation. Internal factors affecting the stability of molecules – dipole interaction, bond opposition strain, bond angle strain. Perspective and Newman projections – representation of different conformations. Conformation of acyclic compounds – Ethane,

n-butane, alkene dihalides,glycols, chloro hydrines, tartaric acid, erythro and threo isomers, aldehydesand ketones (acetaldehyde, acetone).

Interconversion of axial and equatorial bonds in chair conformation – distance between the various H atoms and C atoms in both chair and boat conformations. Monosubstituted cyclohexane – methyl and t-butyl cyclohexanes – flexible and rigid systems. Conformation of disubstituted cyclohexanes (1:1; 1:2; 1:3 and 1:4). Conformation of substituted cyclohexanone-2-bromocyclohexanone, dibromocyclo hexanone, (cis & trans), 2-bromo-4,4-dimethyl cyclohexanone. Anchoring group and conformationaly biased molec ules. 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. Conformations of decaline, adamentane, sucrose and lactos e.

UNIT VI : Conformational Analysis – II (9 h): 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) Action of methyl magnesium bromide on 2-phenylpropionaldehyde (Stereo chemical direction of asymmeetric induction). (d) Dehydrohalogination of stilbenedihalide (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 il lustrated 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) Sem ipinacolic deamination of cis and trans-2-aminocyclohexanol (e) 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 secondary axial and equatorial hydroxyl group to ketones by chronic acid.

UNIT VII : (i) Reactions of Carbon-heteromultiple bonds (7 h): Addition of carbon-oxygen multiple bond: Addition of water, alcohols, amines and hydrazine. Aldol, Perkin, Clainson, Dieckmann, Stobbe and benzoin condensation. Darzons, Knoevenagel, Reforma tosky, Wittig, Cannizaro, Mannich and Prins reactions. MPV reduction and Oppenaur oxidation. Cram's rule. Hydrolysis, alcoholysis and reduction of nitriles. Ritter reactin and Thorpe condensation.

(ii) Esterification and Hydrolysis (2 h) : Mechanism of Ester hydrolysis and esterification, Acyl-oxygen and alkyl oxygen cleavage.

Esterification of axial and equatorial alcohols and acids – their hydrolysis.

References

1. J. March, *Advanced Organic Chemistry*, 4th Edition, John Wiley and Sons, 1992.
2. Morrison & Boyd, Organic Chemistry, Prentice Hall.
3. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry *Parts A & B)*, 3rd Edition, Plenum Press, 1990.
4. E.S. Gould, *Mechanism and structure in organic chemistry*, Holt, Rinehart and Winston, 1959.

UNIT VIII : Introduction to Polymer Chemistry (9 h): Classes of polymers, Synthetic and biopolymers. Synthetic polymers: Chain reaction polymerization and step reaction polymerization. Linear, crosslinked and network polymers. Copolymers, Free -radical and ionic polymerization. Natural and synthetic rubbers.

Biopolymers: Primary, secondary and tertiary structure of proteins, Solid phase peptide synthesis, Protecting groups, Sequence determination of peptides and proteins, Structure and synthesis of glutathione, Structure of RNA and DNA, Structure of cellulose and starch, Conversion of cellulose to Rayon.

References

1. Saunders, *Organic Polymer Chemistry*, Chapman and Hall.
2. S.H. Pine, J.B. Hendrickson, D.J. Cram and G.S. Hammond, *Organic Chemistry*, McGraw Hill International Book Company, 1981.
3. I.L. Finar, *Organic Chemistry*, Vol. II, 5th Edition, ELBS, 1975.
4. Jordean, *The Chemistry of Nucleic Acids*, Buttorworths.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER II

CH2CO4 - THEORETICAL CHEMISTRY II (4 credits)

(72 h)

UNIT I – Foundations of group theory & molecular symmetry (9 h) :
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 II – Representations of point groups & theorems (9 h) :
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} as examples), nomenclature of IR - Mulliken symbols, symmetry species;
Reduction formula - derivation of reduction formula using GOT, reduction of reducible representations, (e.g., Γ_{cart}) using the reduction formula;
Relation between group theory and quantum mechanics – wavefunctions (orbitals) as bases for IR of point groups.

UNIT III Applications of Group Theory to Molecular Spectroscopy (9 h): *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.
Molecular vibrations - symmetry species of normal modes of vibration, construction of Γ_{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.

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

UNIT IV - Applications of Group Theory to Chemical Bonding (9 h) : *Hybridisation* - treatment of hybridization in BF_3 and CH_4, inverse transformation and construction of hybrid orbitals.
Molecular orbital theory - H_2O & BH_3 as examples, classification of atomic orbitals involved into symmetry species, group orbitals, symmetry adapted linear combinations (SALC), projection operator, construction of SALC using projection operator, use of projection operator in constructing SALCs for the π MOs in cyclopropenyl ($C_3H_3^+$) cation.

UNIT V (9 h) : *Basic Principles of Molecular Spectroscopy* - Electromagnetic radiation & it's different regions, interaction of matter with radiation and its effect on the energy of a molecule; Origin of molecular spectra - Theory of the origin of rotational, vibrational and electronic spectra, intensity of spectral lines, dependence of intensity on population, transition probabilities, transition moment integral & selection rules, line widths, Doppler broadening, lifetime broadening.
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.

UNIT VI Infrared & Raman Spectroscopy (9 h) : *Vibrational spectroscopy* - Normal modes of vibration of a molecule; Vibrational spectra of diatomic molecules - harmonic oscillator model, anharmonicity, vibrational transitions and selection rules, 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; Fourier transform infrared (FTIR) spectroscopy (qualitative treatment).
Raman spectroscopy **-** Pure rotational & pure vibrational Raman spectra, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle; Resonance Raman spectroscopy & coherent anti-stokes Raman spectroscopy (basic principles only); Laser Raman spectroscopy.

UNIT VII Electronic spectroscopy (9 h) : *Electronic spectroscopy of Atoms* – The energies of hydrogen atomic orbitals & hydrogen spectrum, coupling of orbital and spin angular momentum, fine structure of H spectrum, The angular momentum of many electron atoms – coupling of angular momenta, LS coupling & J-J coupling, spectroscopic term symbols for atoms, selection rules.
Electronic spectroscopy of molecules - 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; Rotational fine structure of electronic -vibration transitions; Electronic spectra of polyat omic molecules; Electronic spectra of conjugated molecules; Photoelectron spectroscopy (PES) – ultraviolet PES and X-ray PES.

UNIT VIII Spin Resonance Spectroscopy (9 h) : *Nuclear Magnetic Resonance (NMR) spectroscopy* - Magnetic properties of nuclei, the ory and measurement techniques, solvents used, chemical shift and factors influencing chemical shift, shielding effects, spin -spin interaction, coupling constant, factors influencing coupling constant, effects of chemical exchange, fluxional molecules, hin dered rotation on NMR spectrum, Karl's relationships; FTNMR; Principles of 2D NMR spectroscopy - COSY.

Electron Spin Resonance (ESR) spectroscopy - Theory and measurement techniques, g factor, hyperfine interactions, equivalent & non - equivalent protons, Kramer's theorem.

Mossbauer spectroscopy - The Mossbauer effect, hyperfine interactions, isomer shift, electric quadruple and magnetic hyperfine interactions.

Reference

Units I to IV

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.

Units V to VIII

11. G.M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1962.
12. C.N. Banwell & E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, New Delhi, 1994.
13. Thomas Engel, *Quantum Chemistry & Spectroscopy*, Pearson education, 2006.
14. P. Atkins & J. De Paula, *Atkins's Physical Chemistry,* 8th Edition, W.H. Freeman & Co., 2006.

15. D.A. McQuarrie and J.D. Simon, *Physical Chemistry - A Molecular Approach*, University Science Books, 1997.
16. K.J.Laidler, J.H.Meiser and B. C. Sanctuary, *Physical Chemistry,* Houghton Mifflin Company, New York, 2003.
17. D.N. Sathyanarayana, *Electronic Absorption Spectroscopy and Rela ted Techniques*, University Press, 2000.
18. R.S. Drago, *Physical methods in Inorganic Chemistry,* Affiliated East-West Press Pvt. Ltd., 1977.
19. William Kemp, *Organic Spectroscopy*, 3rd Edn., Palgrave, 1991.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER II

CH2CO5 - PHYSICAL CHEMISTRY - I (4 credits), (72 h)

Unit I Electrochemistry – I (9h): Anomalous behavior of strong electrolytes, theory of strong electrolytes, ionic atmosphere, variation of ionic speeds, relaxation time, mechanism of electrol ytic conductance, relaxation and electrophoretic effects, derivation of Debye -Hückel-Onsager equation, deviation from Debye -Hückel-Onsager equation, degree of dissociation and its determination, conductance ratio, Debye - Falkenhagen effect, Wein effect.

Activity and activity coefficients of electrolytes - ionic strength, variation of activity coefficient with concentration; Derivation of Debye - Hückel limiting law and its various forms, qualitative & quantitative verification of the Debye - Hückel limiting law.

Unit II Electrochemistry – II (9h): Polarization - electrolytic polarization, dissolution and deposition potentials, concentration polarization; Decomposition voltage and its determination; Over voltage - hydrogen over voltage, oxygen overvoltage, me tal deposition over voltage and its determination, theories of over voltage; Principles of polarography - dropping mercury electrode, the half wave potential.

UNIT III The Solid State – I (9h): 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 & Herman – Maguin notations, Stereographic projections of the 27 axial point groups, translational symmetry elements & symmetry operations - screw axes and glide planes, introduction to space groups. Imperfections in solids - point, line and plane defects, Non - stoichiometry.

UNIT IV The Solid State – II (9h): Electronic structure of solid s - 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 - Meisner effect, brief discussion of Cooper theory of superconductivity; Optical properties - photo conductivity, luminescence, colour centers, lasers, refraction & birefringence; Magnetic properties - diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism & ferrimagn etism; Thermal properties - thermal conductivity & specific heat.

UNIT V Introduction to Computational Quantum Chemistry (9h) : Classification of computational chemistry methods, ab initio methods - review of Hartree -Fock SCF method, electron correlation, The basis set approximation – use of STOs & GTOs as basis functions, minimal, double zeta, triple zeta, split -valence, polarization & diffuse basis sets, contracted basis sets, Pople -style basis sets and their nomenclature; Model chemistry.

Calculations using Gaussian Programme - Specification of molecular geometry using cartesian coordinates & internal coordinates, The Z - matrix, Z-matrices of some simple molecules (e.g., H_2, H_2O, H_2O_2, ammonia & ethane – eclipsed & staggered conformations), The structure of a Gaussian Input file, Gaussian keywords - OPT and FREQ as examples.

UNIT VI Photochemistry (9h): Photochemical reactions - dimerisation of anthracene, H_2 - Br_2 reaction & H_2 - Cl_2 reactions, photopolymerization; Principles of utilisation of solar energy - solar cells and their working; Photochemical processes - Radiative and non-radiative transitions, chemiluminescence photoluminescence, bioluminescence, thermo - luminescence; Fluorescence - theory of fluorescence, Jablonski diagram, stokes antistokes and resonance fluorescence; Photosensitization - sensitized fluorescence - quenching of fluorescence.

UNIT VII Nuclear and Radiation Chemistry (9h) : Nuclear structure and nuclear stability, Nuclear Models – Fermi gas, collective and optical models; Nuclear reactions: Types, conservation, reaction cross section, compound nucleus theory, specific nuclear reactions, photonuclear and thermonuclear reactions, neutron activation analysis.

Radiation chemistry - interaction of radiation with matter - processes responsible for energy loss, range and range energy relation; Methods of detection & measurement of radiation - principles and working of GM and scintillation counters; Physical and chemical radiation effects in solids, radiation chemistry of water and aqueous ferrous sulphate solutions, radiation hazards and therapeutics, dosimetry.

UNIT VIII (9h): Techniques & instrumentation of IR spectroscopy – single beam and double beam spectrometers, radiation sources, detectors, sample handling; FTIR spectrophotometer Techniques & instrumentation of Raman spectroscopy – radiation sources, detectors, sample handling & illumination.

Techniques & Instrumentation of UV-Visible spectroscopy – radiation sources, filters & monochromators, cells & sampling devices, detectors.

Instrumentation of NMR spectroscopy - Continuous-wave nmr spectrometers – the magnet, the probe unit; Pulsed FTNMR spectrometer.

Reference

Units I & II

1. S. Glasstone, *Introduction to Electrochemistry,* East-West Press Pvt. Ltd., 1965 (Reprint 2008).
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.

Units III & IV

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.
9. A.R. West, *Solid State Chemistry & its Applications,* John Wiley & Sons, 2003 (Reprint 2007).
10. Charles Kittel, *Introduction to Solid State Physics 7th edn*, John Wiley & Sons, 2004 (Reprint 2009).
11. Mark Ladd, *Crystal Structures: Lattices & Solids in Stereoview* , Horwood, 1999.
12. Richard Tilley, *Crystals & Crystal Structures*, John Wiley & Sons, 2006.
13. C. Giacovazzo (ed.) *Fundamentals of Crystallography 2nd edn.*, Oxford Uty. Press, 2002.
14. Werner Massa, *Crystal Structure Determination 2nd edn*., Springer 2004.
15. N.B. Hanna, *Solid state Chemistry,* Prentice Hall.

Unit V

16. C. J. Cramer, *Essentials of computational Chemistry: Theories and models,* John Wiley & Sons 2002.
17. Frank Jensen, *Introduction to Computational Chemistry,* John Wiley & Sons LTD 1999.
18. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
19. Errol G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2nd edn.*, Springer 2011.
20. Thomas Engel & W. Hehre, *Quantum Chemistry and Spectroscopy,* Pearson Education Inc. 2006.
21. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc., 2009.
22. P.W. Atkins & R.S. Friedman, *Molecular quantum mechanics*, 4th Edition, Oxford University Press, 2005.
23. David Young, *Computational Chemistry*, Wiley-Interscience, 2001.

Unit VI

24. C.H. DePuy & O.L.Chapman, *Molecular reactions and Photochemistry* , Prentice Hall, 1972.
25. Alan Cox & James Kemp, *Introductory photochemistry*, McGraw Hill, 1971.
26. P. Suppan, *Chemistry and Light,* RSC London 1994.
27. P. Atkins & J. De Paula, *Atkins's Physical Chemistry,* 8th Edition, W.H. Freeman & Co., 2006.
28. K.J.Laidler, J.H.Meiser and B. C. Sanctuary, *Physical Chemistry,* Houghton Mifflin Company, New York, 2003.
29. G. Raj and H. Misra, *Photochemistry*, Goel Publishing House.

Unit VII

30. Friedlander and J.W. Kennedy, *Introduction to Radiochemistry*, John Wiley & Sons, 1981.
31. S. Glasstone, *Source Book on Atomic Energy*, 3rd *edn*., Affiliated East-West Press Pvt. Ltd., 1967.
32. H.J. Arnikar, *Essentials of Nuclear Chemistry*, 4th edn., New Age International, 1995 (Reprint 2005).
33. W.D.Loveland, D.J.Morrissey, G.T.Seaborg, *Modern Nuclear Chemistry*, Wiley, 2006.
34. G.R.Choppin, J.O.Liljenzin, J.Rydberg, *Radiochemistry & Nuclear Chemistry*, Butterworth-Heinemann, 2002.
35. Kenneth S. Krane, *Introductory Nuclear Physics*, John Wiley & Sons, 1988 (Reprint 2008).
36. D.C. Tayal, *Nuclear Physics 5th edn*., Himalya Publishing House, 2008.

Unit VIII

37. H.H. Willard, L.L. Merritt,Jr., J.A. Dean & F.A. Settle Jr., *Instrumental Methods of Analysis 7th edn.*, CBS Publishers, 1986.
38. C.N. Banwell & E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, New Delhi, 1994.
39. William Kemp, *Organic Spectroscopy, 3rd Edn*., Palgrave, 1991 (Reprint 2005).
40. G.W. Ewing, *Instrumental Methods of Chemical Analysis 5th edn.,* Mc-Graw-Hill, 1985.
41. Robert D Brown, *Introduction to Instrumental Analysis*, PharmaMed Press,1987 (Reprint 2006).
42. G.H. Jeffery, J. Bassett, J. Mendham & R.C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Edition, ELBS, 1989.
43. D.A. Skoog, D.M. West & F. J. Holler, *Fundamentals of Analytical Chemistry*, *8th edn.*, Thomson and Brooks, 2004.
44. D. A. Skoog, F. J. Holler & S. R. Crouch, *Principles of Instrumental Analysis*, Thomson and Brooks, 2007.

UNIVERSITY OF CALICUT
M.Sc. CHEMISTRY (CSS PATTERN) - SEMESTER II
CH2CO6 ORGANIC CHEMISTRY II (4 Credit) (72 hours)

UNIT I: (a) Substitution and elimination reaction (3 hr): Nucleophilic aromatic substitution - Diazonium ion as synthetic intermediate - E1cB Mechanism - Elimination at bridge head carbon - Bredt's rule Chugav reaction.

(b) Free radicals (6 hr): Formation, detection, stability of Free radicals. Free radical addition and substitution reactions – Carbenes and nitrenes (Formation and reactions).

UNIT II: Pericyclic reactions (9 hr): Definition and types of pericyclic reactions - Cycloaddition and cycloreversion, electrocyclic ring closure and ring opening, Sigmatropic rearrangement, ene reactions, Chelotropic reactions. Theoretical models of pericyclic reactions - Orbital correlation method, Transition state aromaticity method, Frontier molecular orbital method. Diel's - Alder Reactions, and Sommelet - Hauser, Cope and Claisen rearrangements. Selection rules and their application to the above reactions.

References:

1. T.H. Lowry and K.S. Richardson, *Mechanism and Theory in Organic Chemistry*, Harpere Collins.
2. S.H. Pine, J.B. Hendrickson, D.J. Cram and G.S.Hammond, *Organic Chemistry,* McGraw Hill International Book Company, 1981.
3. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry (Part A & B)*, 3rd Edition, Plenum Press, 1990.
4. I. Flemming, *Frontier Orbitals and Organic Chemical Reactions,* Wiley, London, 1976.
5. J. Clayden, N. Greeves, S. Warren, and P. Wothers, *Organic Chemistry,* Oxford University Press, 2001.

UNIT III: Molecular Rearrangements and Named reactions (9 hr): Rearrangement involving electron deficient carbon, nitrogen and oxygen atoms. Wagner - Meerwein, Wolff Hoffmann, Beckmann, Schmidt and Baeyer - Villiger, Pinacole-pinacolons, rearrangements.

Anionic rearrangements: Benzil - Benzillic acid, Favorski. Orten - Claisen and Fries rearrangements. Suzuki coupling. Heck, Peterson, Woodward and Prevost hydroxylation reactions.

References:

1. P. Sykes, A guidebook to mechanisms in Organic chemistry, Orient Longmans, 2002.
2. S.H. Pine, J.B. Hendrickson, D.J. Cram and G.S. Hammond, Organic Chemistry, McGraw.
3. J. March, Advanced Organic Chemistry 4th edition John Wiley and Sons, 1992.
4. Jie Jack Li Name reactions 2nd edition.

UNIT IV (9 h) : Spectroscopic Techniques in organic structural determination problem solving approach.

UV-visible: Characteristic absorption of organic compounds - empirical rules for calculating absorption maxima of dienes, enones and aromatic systems.

IR: Characteristic group absorptions of organic molecules - Alkanes, alkenes, alkynes, and aromatic hydrocarbons. Alcohols, phenols, ethers, carbonyl compounds, amines, amides and nitriles.

Optical rotatory dispersion – plain and multiple cotton effect curves - uses. Axial haloketone rule and its application. Octant rule - determination of conformation and configuration of 3-methyl cyclohexanone. ORD curves of cis- and trans- delcalones, circular dichroism curves.

References: IV and V

1. R.M. Silverstein, G.C.Basslar and T.C.Morrill, Spectroscopic identification of organic compounds, John Wiley and Sons, 1991.
2. W. Kemp, Organic Spectroscopy, 3rd edition, M.C.Million, 1991.
3. P.S. Kalsi, Spectroscopy of Organic compound; New age International, 1998.
4. D.L. Pavia; G.M. Lampman and G.S. Kriz; Introduction to spectroscopy, Saunders Golden Sunburst series.
5. W. Kemp and I. Fleming, Organic Spectroscopy.
6. D. Nasipuri, Staeochemistry of Organic Compounds, Wiley Eastern.
7. I.L. Finar, Organic Chemistry, Vol. II, 5th edition, ELBS, 1975.

UNIT V: NMR and Mass spectra (9 h): The chemical shift, local diamagnetic shielding and magnetic equivalence, spin-spin coupling, coupling constant, coupling of protons to other nuclei, quadrupole broading first and second order spectra. Homotopic, enantiotopic and diasterio topic protons. Nuclear overhauser effect (NOE), enhancement simplification of NMR spectra, use of shift reagent High field strength. Spin decoupling and double resonance deuterium labeling and ex change vicinal and germinal coupling in rigid systems. Chemical shift correlation charts proton coupled, offresonence, decoupled and noise decoupled spectra.

Mass spectra: Determination of molecular mass - molecular formulae from isotopic ratio- fragmentation pattern in different classes of compounds. Meta stable ions.

UNIT VI: Synthetic reagents (9 hr): Use of the following reagents in organic synthesis and functional group transformations: Complex metal hydrides - $LiAlH_4$, sodium borohydride and their derivatives, Trimethyl tin hydride, Gilmans reagent Lithium dimethyl cuprate, Lithium dispropyl amide (LDA), Trimethyl silyl chloride, 1,3-Dithiane, Crown ethers, Wilkinson's catalyst, peroxy acids, periodic acids, DCC, DDQ and diborane.

References:

1. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry (Parts A & B),* 3rd Edition, Plenum Press, 1990.
2. H.O. House, *Principles of Organic Synthesis.*
3. J. March, *Advanced Organic Chemistry,* 4th Edition, John Wiley and Sons, 1992.

UNIT VII: Photochemistry (9 hr): Fundamental concepts, molecular excitation, Jablonski diagram and the singlet and triplet states photosensitization. Reaction involving the olefinic double bonds, reactions of carbonyl compounds and reactions of aromatic compounds. Di-π-methane rearrangement Barton reaction and Photofries rearrangement photopolymerisation and photochemical degradation of polymers photochemistry of dyes and pigments.

References:

1. R.O.Kan Organic Photochemistry, McGraw Hill.
2. O.L. Chapman, Organic photoche mistry, Vol.I & II, Marcel Decker.

UNIT VIII: Chemistry of Natural Products (9 hr): Chemical classification of Natural products classification of alkaloids based on ring structure, Isolation and general methods of structure elucidation based on degradative reactions. Structure of atropine -synthesis of quinine.

Terpenoids - Isolation and classification of terpenoids, structure of steroids classification of steroids, Woodward synthesis of cholesterol conversion of cholesterol to testosterone. Flavones a nd Isoflavones - synthesis only.

References:

1. I.L. Finar, Organic Chemistry, Vol. II, 5 th Edition, ELBS, 1975.
2. P.S. Kalsi, Chemistry of Natural products, Wiley Eastern.

UNIVERSITY OF CALICUT
M.Sc. CHEMISTRY – SEMESTER I & II

CH1PO1 & CH2PO1 – INORGANIC CHEMISTRY PRACTICALS – I
(4 Credits)

UNIT I

Separation and identification of four metal ions of which two are less familiar elements like W, Se Te, Mo, Ce, Th, Ti, Zr, V, U and Li. (Eliminating acid radicals not present). Confirmation by spot tests.

UNIT II

Volumetric Determinations using:

(a) EDTA (Al, Ba, Ca, Cu, Fe, Ni, Co, hardness of water)

(b) Cerimetry (Fe^{2+}, nitrite)

(c) Potassium Iodate (Iodide, Sn^{2+})

UNIT III

Colorimetric Determinations of metal ions

Fe, Cr, Ni, Mn and Ti.

References

1. G.H. Jeffery, J. Basseett, J. Mendham and R.C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Edition, ELBS, 1989.

2. D.A. Skoog and D.M. West, *Analytical Chemistry, An Introduction*, 4th Edition, CBS Publishing Japan Ltd., 1986.

3. E.J. Meehan, S. Bruckenstein and I.M. Kolthoff and E.B. Sandell, *Quantitative Chemical Analysis*, 4th Edition, The Macmillan Company, 1969.

4. R.A. Day (Jr.) and A.L. Underwood, *Quantitative Analysis*, 6th Edition, Prentice Hall of India, 1993.

UNIVERSITY OF CALICUT
M.Sc. CHEMISTRY – SEMESTER I & II

CH1PO2, CH2PO2 – ORGANIC CHEMISTRY – I (4 Credits)

UNIT I : Laboratory Techniques

Methods of Separation and Purification of Organic Compounds – fractional, steam and low-pressure distillations, fractional crystallisation and sublimation.

UNIT II : Separation and identification of the components of organic binary mixtures.

Analysis of about ten mixtures, some of which containing compounds with more than one functional group.

UNIT III : Organic preparations-double stage (minimum six)

References

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, ELBS/Longman, 1989.
2. Shriner, Fuson and Cartin, *Systematic Identification of Organic Compounds*, 1964.
3. Fieser, *Experiments in Organic Chemistry*, 1957.
4. Dey, Sitaraman and Govindachari, *A Laboratory Manual of Organic Chemistry*, 3rd Edition, 1957.
5. P.R. Singh, D.C. Gupta and K.S. Bajpal, *Experimental Organic Chemistry*, Vol. I and II, 1980.
6. Vishnoi, *Practical Organic Chemistry*.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (I & II Semesters)

CH1PO3, CH2PO3 - Physical Chemistry Practical – I (4 credits)

SECTION A

UNIT I. Solubility and Heat of solution (minimum 2 experiments)

1. Determination of molar heat of solution of a subst ance (e.g., ammonium oxalate, succinic acid) from solubility data - analytical method and graphical method

UNIT II. Phase Equilibria (minimum 3 experiments)

1. (a) Determination of phase diagram of a simple eutectic system (e.g., Naphthalene – Biphenyl, Naphthalene-Diphenyl amine)
   (b) Determination of the composition of a binary solid mixture.
2. Determination of phase diagram of a binary solid system forming a compound (e.g., Naphthalene – m-dinitrobenzene).

UNIT III. Viscosity (minimum 2 experiments)

1. Viscosity of mixtures - Verification of Kendall's equation (e.g., benzene - nitrobenzene, water-alcohol).
2. Determination of molecular weight of a polymer (e.g., polystyrene in toluene).

UNIT IV. Distribution Law (minimum 3 experiments)

1. Determination of distribution coefficient of I_2 between CCl_4 and H_2O.
2. Determination of equilibrium constant of $KI + I_2 = KI_3$
3. Determination of concentration of KI solution

SECTION B

UNIT V - Refractometry (minimum 3 experiments)

1. Determination of mola r refractions of pure liquids (e.g., water, methanol, ethanol, chloroform, carbon tetrachloride, glycerol)
2. Determination of composition of liquid mixtures (e.g., alcohol -water, glycerol-water)
3. Determination of molar refraction and refractive index of a sol id substance

UNIT VI - Conductivity (minimum 4 experiments)

1. Determination of equivalent conductance of a weak electrolyte (e.g., acetic acid), verification of Ostwald's dilution law and calculation of dissociation constant.
2. Determination of solubility product of a sparingly soluble salt (e.g., AgCl, $BaS0_4$)
3. Conductometric titrations
   (a) HCl vs NaOH
   (b) (HCl + CH_3 – COOH) vs NaOH
4. Determination of the degree of hydrolysis of aniline hydrochloride

UNIT VII - Potentiometry (minimum 3 experiments)

1. Potentiometric titration: HCl vs NaOH, CH_3-COOH vs NaOH
2. Redox titration: KI vs $KMnO_4$, $FeS0_4$ vs $K_2Cr_2O_7$
3. Determination of dissociation constant of acetic acid by potentiometric titration

References

1. A. Finlay, *Practical Physical Chemistry*, Longman's Green & Co.
2. J.B. Firth, *Practical Physical Chemistry*, Read Books (Reprint 2008).
3. A.M. James, *Practical Physical Chemistry*, Longman, 1974.
4. F. Daniel, J.W. Williams, P. Bender, R.A. Alberty, C.D. Cornwell and J.E. Harriman, *Experimental Physical Chemistry*, McGraw Hill, 1970.
5. W.G. Palmer, *Experimental Physical Chemistry*, 2nd Edition, Cambridge University Press, 1962.
6. D.P. Shoemaker and C.W. Garland, *Experimental Physical Chemistry*, McGraw Hill.
7. J. B. Yadav, *Advanced Practical Physical Chemistry, Goel Publications,* 1989.
8. B. Viswanathan & R.S. Raghavan, *Practical Physical Chemistry*, Viva Books, 2009.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER III

CH3CO7 - PHYSICAL CHEMISTRY II (4 credits)

(72 h)

UNIT I - Statistical Mechanics - I (9 h): 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 mac rostates, 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 t he thermodynamic properties; Evaluation of partition functions and thermodynamic properties for ideal mono -atomic and diatomic gases.

UNIT II - Statistical Mechanics - II (9 h): Heat capacities of solids - classical and quantum theories, Einstein's theo ry of atomic crystals and Debye's modification.

Heat capacities of gases - classical and quantum theories, the anomalous heat capacity of hydrogen, ortho and para hydrogens.

UNIT III Statistical Mechanics III (9 h): *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.

The liquid state - Structure of liquids, X-ray diffraction studies of simple liquids, short range order, radial distribution function, configurational partition function for liquids, theories of liquids - free volume theory & simple hole theory, communal entropy in liquids.

UNIT IV Thermodynamics of Irreversible Processes (9 h): Simple examples of irreversible processes, general theory of non -equilibrium processes, entropy production, the phenomenological relations, Onsager reciprocal relations, application to the theory of diffu sion, thermal diffusion, thermo-osmosis and thermo-molecular pressure difference, electro-kinetic effects, the Glansdorf-Pregogine equation.

UNIT V – Chemical Kinetics (9 h) : *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 VI – Molecular Reaction Dynamics (9 h): *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 VII – Surface Chemistry (9 h): Adsorption: Adsorption isotherms, Langmuir's unimolecular theory of adsorption, Statistical derivation of Langmuir isotherm. BET equation, derivation, determination of surface area of adsorbents, heat of adsorption and its determination; Experimental methods for studying surfaces - Principles of SEM, STM, ESCA & Auger spectroscopy.

UNIT VIII – Catalysis (9h): 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 $2CO + O_2 \rightarrow 2CO_2$

Reference

Units I to IV

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. J.A. Berker, *Lattice theories of liquid states*, Pergamon Press.
7. G.K. Vemulapalli, *Physical Chemistry*, Prince Hall India.
8. M.C. Guptha, *Statistical Thermodynamics*, Wiley eastern Ltd., 1993.
9. S. Glasstone, *Thermodynamics for Chemists*, East-West, 1973
10. Pigoggine, *An introduction to Thermodynamics of irreversible processes*, Interscience

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

Units V & VIII

1. P. Atkins & J. De Paula, *Atkins's Physical Chemistry,* 8th Edition, W.H. Freeman & Co., 2006.
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

UNIVERSITY OF CALICUT
M.Sc. CHEMISTRY (CSS PATTERN) SEMESTER III

CH3CO8 - INORGANIC CHEMISTRY II (4 Credits) (72 h)

Unit I (9 hr): Electronic spectra of complexes, Term of d^n configurations, selection rules. Effect of ligand field on RS terms. Orgal diagram and its uses. Tanabe-Sugano diagrams, Charge transfer spectra, Spectra of f-block complexes.

Unit II (9 hr): Magnetic properties of metal complexes - types of magnetic properties paramagnetism and diagmagnetism - Curie an Curie-Weiss law. μ, μ_{1+s} and spin only expressions. Orbital magnetic moment and its quenching, Spin-orbit coupling. Temperature independent paramagnetism. Spin cross over in coordination complexes, magnetic properties of f-block elements. Ferro and antiferro magnetic interactions. Determination of magnetic moment - Gouy method.

Unit III (9 hr): Reaction mechanisms of metal complexes. Classification, Rate laws, Substitution reactions in octahedral complexes. A, D and I mechanisms. Aquation and base hydrolysis, Fuoss - Eigen equation. Substitutions in square planar complexes. Trans effect - theories and applications. The cis-effect.

Unit IV (9 hr): Redox raction mechanism, classification, outer sphere and inner sphere electron transfer. Marcus equation. Bridging group effects, photochemical reactions of metal complexes. Photosubstitution, photoaquation and ligand exchange reactions - metal complex sensitizers, photochemical reactions of chromium and ruthenium complexes.

Unit V (9 hr): Infrared spectra of metal complexes, -Group frequency concept. Changes in ligand vibrations on coordination - metal ligand vibrations. Application to coordination compounds - IR spectra of metal carbonyls - ESR spectra- application to copper complexes, Mossbauer spectra - application to iron complexes - Application of NMR spectra of diamagnetic complexes.

Unit VI (9 hr): Organometallic compounds I - Classification and nomenclature, Carbon σ- donors, Alkyls and aryls of main group metals- synthesis, structure, bonding and applications. Organometallic compounds of transition metals. The 18 electron rule, syntheses, structure and bonding in metal carbonyls, carbenes, carbynes.

Unit VII (9 hr): Organometallic compounds II - Coordination of transition metals to carbon multiple bonds, synthesis, structure, bonding and applications of complexes of ethylene, allyl, butadiene and acetylenes. Synthesis, structure, bonding and reactions of typical transition metal complexes of C_4H_4, $C_5H_5^-$ C_6H_6 and $C_8H_8^{2-}$

Unit VIII (9 hr): Introduction to bioinorganic chemistry, occurrence of inorganic elements in biological system, bulk and trace metal ions, coordination sites in biologically important ligands. Effect of the nature

of metal ions and ligand on the stability of the complexes. Role of sodium, potassium and calcium in biological system. Metalloenzymes : Zn(II) containing enzymes, iron enzymes, peroxidase, copper enzymes - oxidase, tyrosinase, superoxide dismutase, Vitamin B_{12} and coenzymes. Cytochromes and iron-sulphur proteins. Nitrogenases, biological nitrogen fixation, chlorophyll-photosystem 1 and I.

References:

1. D.F. Shriver, P.W. Atkins and C.H. Langford, *Inorganic Chemistry,* ELBS, 1990.
2. J.E. Huhey, E.A. Keiter and R.L. Keiter, *Inorganic Chemistry*, *Principles, Structure and Reactivity, Pearson Education* , 2001.
3. F.A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry,* Wiley.
4. R.S. Drago, *Physical methods in Inorganic Chemistry,* Affiliated East-West Press Pvt. Ltd., 1977.
5. R.L. Dutta and A. Shyamal, *Elements of Magnetochemistry*, S. Chand & Co., 1982.
6. A. Earnshaw, *Introduction to Magnetochemistry,* Academic Press, 1968.
7. D. Sutton, *Electronic Spectra of Transition Metal Complexes,* McGraw Hill, 1968.
8. J.C. Blair Jr. (Ed.)., *The Chemistry of Coordination Compounds*, Reinhold Pub. Cor., 1960.
9. L.F. Lindoy, *The Chemistry of Macrocyclic Ligands and Complexes,* Cambridge University Press, 1989.
10. G.Wulfsberg, *Inorganic Chemistry,* University Science Books, 2000.
11. Holleman- Wiberg, *Inorganic Chemistry,* Academic Press, 1995.
12. G.L. Miessler and D.A. Tarr, *Inorganic Chemistry,* Person Education, 2004.
13. P. Powell, *Principles of Organometallic Chemistry*, 2nd Edition, ELBS, 1988.
14. R.C. Mehrothra and A. Singh, *Organometallic Chemistry, A Unified Approach*, Wiley Eastern, 1991.
15. R.W. Hay, *Bioinorganic Chemistry*, Ellis Horwood Ltd., 1984.
16. D.E. Fenton, *Biocoordination Chemistry,* Oxford University Press, 1995.
17. L.F. Lindoy, *The Chemistry for Macrocyclic Ligands and Complexes,* Cambridge Books, 1994.
18. S.J. Lippard and J.M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, 1994.
19. I. Bertin, H.B. Gray, S.J. Lippard and J.S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., 1998.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER III

CH3EO1 Synthetic Organic Chemistry (Elective) (4 credits)

UNIT I: Formation of Carbon-Carbon bond (9 hr): Carbon- Carbon bond formation via Electrophitic and nucleophilic carbon species. Base catalysed condensations, Mannich base as intermediates in organic synthesis, four centre reaction- Diel's Alder reaction, 1,3-dipolar additions.

References:

1. R.O.C. Norman, Principles of Organic Synthesis.
2. R.K. Michael and B. Smith, Organic synthesis.
3. Hendrickson, Cram and Hammond, Organic Chemistry.
4. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part B, 3 rd Edition, Plenum Press.
5. S. Warren, Organic Synthesis, The Disconnection Approach, John Wiley.

UNIT II (9 hr): (i) Formation of Carbon-Nitrogen Bond (9 hr): Nucleophilic nitrogen and electrophilic carbon, Electrophilic nitrogen and nucleophilic carbon skrarp synthesis, Bischler- Napiaralski reaction.

(ii) Formation of Carbon-Halogen Bond: Allylic halogenation by NBS, NCS and NIS photochemical methods of organic synthesis (suitable example).

References:

1. R.O.C. Norman, Principles of Organic Synthesis.
2. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part B, 3 rd Edition, Plenum Press.
3. R.K. Michael and B. Smith, Organic Synthesis.
4. J. March, Advanced Organic Chemistry, 4 th edition, John Wiley and Sons, 1992.

UNIT III: Reduction and Oxidation (9 h): Catalytic hydrogenation, Metal hydride reductions, dissolving metal reductions. Reduction of specific functional group- reduction of alkenes, alkynes of aldehydes and ketones to alcohols. Ketones to methylene group reductive ring opening of epoxides. Reduction of unsaturated carbonyl compounds, reduction of aromatic and heterocyclic compounds.

Oxidation with transition metal oxidants (Cr, Mn) Oxygen, O_3, and peroxides, lead tetra acetate and ScO_2 oxidation of carbon- carbon double bonds, alcohols, glycols, ketones, and aldehydes, allylic oxidation, oxidative-decarboxylation.

References:

1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1987.

2. H.O. House, Modern Synthetic Reaction, W.A. Benjamin, 1965.

UNIT IV: Reagents in Organic Synthesis (9 hr) : Use of the following reagents in organic synthesis and functional group transformation complex metal hydrides, Gilman's reagent, Tri -n-butyl tin hydride, organometallic reagents of Alumi nium, Cadmium, Zinc, and Fe. Benzene Tricarbonyl Chromium , preparation and reaction with carbanions.

References:

1. Fieser and Fieser, Reagents in Organic Synthesis.
2. S.G. Daus, Organotransition metal chemistry applicati on to Organic Synthesis, Pergman Press, London, 1982.
3. H.O. House, Modern Synthetic Reactions.
4. W. Carnethers, Some modern methods of Organic Synthesis, Benjamin Publications, California, 1972.
5. V.K. Ahluwalia and R. Agarwal Organic Synthesis, Specia l techniques, Narose.
6. M.B. Smith, Organic Synthesis, 2nd edition, McGraw Hill.
7. P.R. Jenkins, Organometallic reagents in synthesis, Ou primer 3 oup.

UNIT V: Multi step Synthesis (9 hr): Synthetic analysis and planning, Elements of a Synthesis (Reacti on methods, reagents, catalysts, solvents, protective groups for hydroxyl, amino, Carbonyl and carboxylic acids, activating groups, leaving groups synthesis and synthetic equivalents. Types of selectivities (Che mo, regio, stereo selectivities) synthetic planning illustrated by simple molecules, disconnections and functional group interconversions, uplong reactions and use in synthesis, Retrosynthetic analysis of a complex molecule - a case study.

References:

1. John McMurry, Organic Chemistry, 5th Edition, 2000, or newer.
2. Stuart Warren Designing, Organic Synthesis, Programmed introduction to the synthesis approach, 1994.
3. Classics in Total synthesis K.C.Nicolaou, E.J. Sorenson, VCH, 1996.
4. Organic synthesis, Micheal Smith, 2nd Edition, McGraw Hill, 2004.
5. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry Part B, 3rd Edition, Plenum Press.
6. R.O.C. Norman, Principles of Organic Synthesis.

UNIT VI: Synthesis of Natural Products (9 hr) : Synthetic studies on Longifolene, Reserpine, Prostaglande n E, Cephalosporin, Vitamin A.

References:

1. I. Fleming, Selected Organic Synthesis, John Wiley and Sons, 1982.
2. T. Landbery, Strategies and Tactics in Organic Synthesis, Academic Press, London,1989.
3. E. Corey and I.M. Chang, Logic of Chemical Synthes is, John Wiley, New York, 1989.

4. I.L. Finar, Organic Chemistry, Vol. II, 5th Edition, ELBS, 1925.

UNIT VII: Palladium Catalysed Coupling Reaction (9 h): Palladium Catalysts 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).

References:

1. Metal Catalysed cross coupling reactions, Dieckrich, F and Stang P.J, Eds., Wiley, VCH, New York, 1988.
2. V. Farine, V, Krishnamurthy, Scott W.J., The stille reaction, John Wiley and Sons, New York, 1998.
3. Lazzlo Kurti and Barbosa Czako, Strategic application of Named reactions in Organic synthesis, Elcener Academic Press, 2005.

UNIT VIII: Heterocyclic compounds (9 hr): Aromatic and nonaromatic heterocyclic, common structured types, structure, synthesis and reactions of oxazole, pyrazole, imidazole and thiazole synthesis of uracol, thymine and cytosine. Synthesis of adenine and guanine. Synthesis of uric acid, caffene, pyrazine, synthesis of furanones, tetrazole.

References:

1. I.L. Finar, Organic Chemistry, Vol.II, 5th Edition, ELBS, 1975.
2. Acheson, An introduction to the chemistry of Heterocyclic compounds, Interscience, 1960.
3. Badger, The Chemistry of Heterocyclic Compounds, Academic Press, 1961.

UNIVERSITY OF CALICUT
M.Sc. CHEMISTRY (CSS PATTERN) SEMESTER III

CH3EO2 : NATURAL PRODUCTS (Elective) (4 Credits)

UNIT I: (9 hr): (i) Taxonomy of Plants: Location, identification, cultivation, collection, storage and uses of the following medicinal plants - Ocimum sanctum, Phyllanthus, adathoda Vasica and Rawolfia se rpentina.

(ii) Classification of Natural Products : Classification of Natural products based on chemical structure, physiological activity, taxonomy and Biogenesis. Carbohydrates, Terpenoids, Carotenoids, alkaloids, steroids, anthocyanins etc. Methods of isolation of each class of compound.

References:

1. V.V. Sivarajan and Manilal K.S., *Flora of Calicut.*
2. Hill, *Economic Botany.*
3. Lawrence, *Taxonomy of Vascular Plants,* New Delhi, 1974.
4. A.B. Rendle, *The Classification of Flowering Plants,* Cambridge University Press, 1871.
5. J.S. Gamble, *Flora of the Presidency of Madras,* Bot. Survey of India, Calcutta, 1957.
6. Koji Nakanishi, Toshio Goto, Sho Ito, Shinsaku Natori, and Shige Nozoe (Eds.), *Natural Products Chemistry*, Vol. I, Kodansha Scientific Ltd., 1974.
7. N.R. Krishnaswamy, Natural Products Chemistry, Oxford University Press.

UNIT II: Terpenoids (9 hr) : Methods of isolation, Classification and general structure elucidation of terpenoids, isoprene rule. Synthesis of Lupeol and β-amyrin, structure elucidation of Farnesol and Menthol, stereochemistry of camphor and abeitic acid.

References:

1. P. De Meyo, *The higher Terpenoids.*
2. A.R. Pinder, *The Chemistry of Terpenes.*
3. Simonson, Terpenoids.
4. A.A. Newman (Ed.), *The Chemistry of Terpenoids.*
5. I.L. Finar, *Organic Chemistry,* Vol.II, 5th edition, ELBS, 1975.

UNIT III: Steroids (9 hr): Classification and isolation of steroids. Detailed study including structure elucidation, synthesis and stereo -chemistry of the following.

Cholesterol, Ergosterol, Ergocalciferol, Oesterone, Diosgenin, Oestradiol, Oestriol, Equilenine, Androsterone, Testosterone, Progestrone, Bile acids, Cholic acid, Cortisone and Corticosterone.

References:

1. Fieser and Fieser, *Steroids,* Asia Publishing House, 1959.
2. Klyne, *The chemistry of steroids.*

3. Shoppe, Chemistry of the steroids.
4. Templeton, *An Introduction to the Chemistry of the Terpenoids and Steroids.*
5. I.L. Finar, *Organic Chemistry,* Vol.II, 5th Edition, ELBS, 1975.

UNIT IV: Alkaloids (9 hr): Nomenclature, classification, isolation, chromatography and other techniques of purification. D etailed study of the following. Morphine, Reserpine, Tylophorin and Lysergic acid.

References:

1. K.W. Bentley, *Alkaloids,* Interscience Publishers, 1965.
2. R.H.F. Maniske and H.L. Holmass, *The Alkaloids-chemistry and Physiology,* Academic Press Inc., 1952.
3. Henry, *The Plant Alkaloids.*
4. Koji Nakanishi, Toshio Goto, Sho Ito, Shinsaku Natori, and Shige Nozoe (Eds.), *Natural Products Chemistry*, Vol. I, Kodansha Scientific Ltd., 1974.
5. I.L. Finar, *Organic Chemistry,* Vol.II, 5th Edition, ELBS, 1975.

UNIT V (9 hr): (i) Anthocyanins: Introduction, General Nature and Structure of Anthocyanidins. Flavone, Flavonol, Quercetin, Isoflavone (Daidezein) and Chalcone.

References:

1. Bentley, *The Natural pigments,,* Interscience.
2. Geissman (ed.), *The Chemistry of Flavonoid Compounds,* Pergamon.
3. Bernfell (ed.), *Biogenesis of Natural Compounds,* Pergamon.
4. Harborne, *Comparative Biochemistry of Flavonoids,* Academic Press, 1967.
5. I.L. Finar, *Organic Chemistry,* Vol. II, 5th Edition, ELBS, 1975.

(ii) Prostaglandins: Chemistry of Prostagiandins - Isolation, Classification, Structural elucidation and Synthesis of PGE, PGF, PGA and PGB groups of prostaglandins.

References:

1. S.H. Pine, J.B. Hendrickson, D. J. Cram and G.S. Hammond, *Organic Chemistry,* McGraw Hill International Book Company, 1981.
2. Koji Nakanishi, Toshio Goto, Sho Ito, Shinsaku Natori, and Shige Nozoe (Eds.), *Natural Products Chemistry*, Vol. I, Kodansha Scientific Ltd., 1974.

UNIT VI (9 hr): (i) Application of IR, UV, NMR, Mass, CD and ORD in the structural elucidation of Natural products.

References:

1. *Determination of Organic Structure by Physical Methods,* Vol.I to IV, Academic Press.
2. Schwarz (Ed.), *Physical Methods in Organic Chemistry,* Oliver and Boud, 1964.
3. Djersassi, *Optical Rotatory Dispersion,* McGraw Hill, 1960.

4. Crabbe, *Optical Rotatory Dispersion and Circular Dichroism in Organic Chemistry,* Holdern Day, 1965.
5. William and Fleming, *Spectroscopic methods in Organic Chemistry,* McGraw Hill, 1966.
6. Bible, *Interpretation of NMR spectra,* Plenum Press, 1965.

ii) Haemin and Chlorophyl: Structure and synthesis of Porphyrins, Chemistry of Haemin and Chlorophyl.

References:

1. I.L. Finar, *Organic Chemistry,* Vol. II, 5th edition, ELBS, 1975.
2. D. Nelson and M. Cox, *Leneinger's Principles of Biochemistry,* Worth Publishers, New York.

UNIT VII: Essential Oils and Aromatics (9 hr): Isolation and study of important constituents of lemon grass oil, citronella oil, agowan oil, cinnamon oil, palmarosa oil, rosemary oil, patchouli oil, peppermint oi l, turpentine oil, clove oil, sandalwood oil, lavender oil, rose oil. Essential oils of turmeric and ginger. Oleoresins of pepper, chilly, ginger and turmeric, use of essential oil in medicine - Aromatherapy.

References:

1. The essential oils, The constitu ent of essential oils by Ernest Guenther, 1975.
2. Organic Chemistry by I.L. Finar, Vol. II.

UNIT VIII: Vitamins (9 hr): Occurrence, isolation, biological significance (brief idea) and synthesis of the following vitamins : Vitamin A, E, K, Thiamine, Riboflavin, Pyridoxine, Niacin, Pantothenic acid and ascorbic acid.

References:

1. Organic Chemistry by I.C. Finar, Vol. II.
2. Chemistry of Natural Products by Bhat, Nagasampagi and Sivakumar, 2005, Narosa Publishing.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER III

CH3EO3. Polymer Chemistry (Elective) (4 Credits)

UNIT I: Methods of Polymerization (9 hr) : Step reaction (Condensation) Polymerization: Mechanism, types and Kinetics of condensation polymerization. Interfacial condensation. Ring verses chain formation. Bifunctional and Polyfunctional step reaction polymerization - gelation, gelpoint- experimental, observation, Molecular weight distribution, Ring scission polymerization.

Radical Chain (Addition) Polymerization: Vinyl polymerizat ion, Vinyl monomers, Mechanism of Vinyl polymerization, Experimental methods in Vinyl polymerization. Kinetics of free radical polymerization, Degree of polymerization-chain transfer. Molecular weights and its distribution. Effect of temperature and pre ssure on chain polymerization.

Ionic Polymerization: Anionic polymerization - Initiation and Propagation Mechanisms, Kinetics, Living polymerization, Ionic equilibrium. Molar mass distribution. Transfer and termination, stereocontrol, cationic polymeriza tion- Mechanis, Kinetics, Radiation activated polymerization.

UNIT II: Method of Polymerization II (9 hr): Suspension and emulsion polymerization of mono and hetrodisperse polymers.

Co-ordination Chain Polymerization: Ziegler - Natta Catalysis. Mechanism, Kinetics - Ring opening polymerization.

Co-polymerization: Different types of copolymers, kinetics of co - polymerisation (Free radial and Ionic). The co -polymerization equations, composition of copolymers, Mechanism of co -polymerization - Monimer reactivity ratios and co-polymerisation parameters. Chemistry of co-polymerization, Reactivity and structure of monomers and radicals. Polymerization in homogenous and heterogeneous systems. Gas phase polymerization, Bulk polymerization and polymer precipitate.

UNIT III: Chemical reactions of polymers (9 hr) : Basic principles, Molecular and chemical groups. Reactivity of functional groups. Post reactions of polymers - Chain Extension, Branching and gross linking reactions, polymer analogues reactions. Polym er Degradation reactions, Polymer blends, Functionalization of polystyrene. Preparation of ion exchange resins, polymer -bound reagents, immobilized enzymes. Solid phase peptide synthesis (SPPS) merits and demerits.

UNIT IV: Classification of Polymers (9 hr): Plastics, rubbers and fibers, thermosets and thermoplastic, linear, branched and cross -linked

polymers, random, block and graft co-polymers and stereo specific polymers.

UNIT V: Polymer Solutions (9 hr): General role of polymer solubility parameters Flory-Huggins treatment of polymer solution, enthalpy, entropy an free energy change in polymer dissolution. Unperturbed chain dimension, viscosity of polymer solution, osmotic pressure, swelling of polymers, fractionation of polymers, phase separation in polymers.

UNIT VI (9 h): Studies on the thermal, optical, electrical and mechanical properties of polymers, correlation of structure to these properties. First order and second order transition points. Glass transition temperature, Melting temperature- Experimental method of their determinations.

Method of molecular weight determination of polymers. End-group analysis, colligative property measurement, concentration dependence of colligative properties, Vapour pressure lowering, cryoscopy and osmometry, Light-scattering methods. Ultra centrifugation, Solution viscosity and molecular size, experimental methods, treatment of data, staudinger index, empirical correlations between intrinsic viscosity and molecular size of polymer structure. Gel permeation chromatograph and other chatographic techniques in the fractionation polymers.

UNIT VII: Polymer Degradation (9 hr): Mechanism of Polymer degradation. Thermal, mechanical and photochemical degradations. Oxidation and ozone attack. Acid and base hydrolysis, Bio-degradation of polymers.

UNIT VIII: Structure and applications of the following (9 hr) :

a) Cellulose and cellulose based polymers- Native and modified cotton Rayon. Cellulose nitrate, cellulose acetate.

b) Polyolefins- Polyethylene and Polypropylene.

c) Vinylpolymers- PVC, Polystyrene, acrylic polymers.

d) Flurocarbon polymers- Teflon.

e) Phenol formaldehyde and urea formaldehyde resins.

f) Polyamides (Nylon) and Polyesters (Terylenes)

g) Carprolactam based polymers.

References

1. F.W. Billmeyer, Text Book of Polymer Science, Wiley-Inter Sciences (1976).
2. G.Odian, 'Principles of Polymerization', McGraw Hill, 1970.
3. Eiias, 'Macromolecules' Plenum Press, 1980.
4. M.L. Miller, The structure of Polymers Reinhold, 1968.
5. C.M. Blow and C.Hephrun (eds.) 'Rubber Technology and Manufacture', Buthesworthes, 1982.
6. I.M. Campbell, 'Introduction to polymers', Oxford Scientific Publications, 1994.
7. K. J. Saunders, 'Organic Polymer Chemistry Chapman and Hall, London, Mathur, Narang and Williams, 'Poly mers as Aids in Organic Chemistry, Academic Press, London.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER IV

CH4CO9 Advanced Topics in Chemistry (4 Credits)

UNIT I : Metal Clusters (9 h): Metal-metal bonds and metal clusters - single, double, triple and quadruple bonded non-carbonyl clusters. The isolobal analogies cluster structure and electron count. The Wade - Mingos- Lauher rules, Higher carbonyl clusters.

UNIT II : Reaction pathways of Organometallic compounds (9 h): Oxidative addition and reductive elimination - mechanism, Oxidative coupling and reductive cleavage. Insertion reactions involving CO, NO, Isocyanide, alkenes, alkynes, CO_2 and SO_2. α, β eliminations. Nucleophilic additions and abstractions to coordinated legends such as CO, polyenes, alkyls and acyls Electrophelic addition and abstraction to alkyl groups. Carbonylation by Collman's reagent.

UNIT III : Catalysis by organometallic complexes (9 h): Alkene hydrogenation, isomerisation, hydroboration and hydroformylation of alkenes, Monsanto acetic acid process, Wacker process Dimerization, Oligomerization and Polymerization, Fischer-Trops reaction, Watergas shift reaction.

UNIT IV : Medicinal Chemistry (9 h): Drugs: Introduction, different classes of drug, drug action, drug design, prodrugs, factors governing drug design, rational approach to drug design, SAR and QSAR, physico - chemical factors and biological activities, factors governing ability of drugs. General methods of drug synthesis. Analgesics (Phenazones and Phenylbutzone as examples), Antipyretic (Paracetamol), Antibiotics, Pencillins, Chloramphanicol.

UNIT V – Green Chemistry (9 h): 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 with classical reactions; Green preparations, Applications phase transfer catalysts, Introduction to Microwave organic synthesis, Applications: environmental, solvents, time and energy benefits.

UNIT VI – Nanoscience and Technology (9 h): Introduction, nanostructures: tubes, fibers, wires, bricks and building blocks, nanostructure formation: lithography, self-assembly,molecular synthesis,crystal growth and polymerization, measurement of nanostructure: spectroscopy,microscopy and electrochemistry, nano CAD.

UNIT VII - Nanomaterials (9 h): Nanocomposites, consumer goods, 'smart materials,' Applications to various fields:optics, telecommunication, electronics, digital technology and environment, Biomedical applications: diagnosation, protic engineering, mapping of genes, drug delivery, biomimetics, quantum dots.

UNIT VIII – Supramolecular Chemistry (9 h): *Molecular recognition:* Receptors, design and synthesis of co-receptors and Multiple recognition, Hydrogen bonds, strong, weak and very weak H-bonds, Utilisation of H-bonds to create supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition .

Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules. Supramolecular reactivity and catalysis. Transport processes and carrier design. Supramolecular devices, supramolecular photochemistry. Novel liquid crystals, Gelators fibres and adhesives, Dendrimers, organic solids, organic conductors and organic superconductors, catenanes and rotaxanes

References

1. F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley, Chichester, 1999.
2. J.N. Delgado and W.A. Remers, (Ed.), *Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry*, 10th Edition, Lippincott – Raven Publishers, 1998.
3. Harkishan Singh and V.K. Kapoor, *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, 2008.
4. G. Thomas, *Fundamentals of Medicinal Chemistry*, Wiley.
5. A. Gringauz, *Introduction to Medical Chemistry*, Wiley – VCH, 1997.
6. P.T. Anastas and J.C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, Oxford, 1998.
7. James Clark and Duncan Macquarrie, *Handbook of Green Chemistry and Technology*, Blackwell Science, 2002.
8. J.H. Clark, *The Chemistry of Waste Minimization*, Blackie Academic, London, 1995.
9. Jeiping Zhu and Hugues Bienayme (Ed.), *Multi Component Reactions*, Wiley VCH Velag GmbH & Co., KGaA, Weinheim, 2005.
10. J.M. Martinez Durat, R.J. Martin Palma and F. Agullo Rueda, *Nanotechnology for Microelectronics and Optoelectronics,* Elsevier, 2003.
11. G.A. Ozin and A.C. Arsenault, *Nanochemistry*, RSC Publishing, 2008.
12. C.P. Poole (Jr.) and F.J. Owens, *Introduction to Nanotechnology*, Wiley, 2007.
13. F. Vögtle, *Supramolecular Chemistry*, John Wiley & Sons, Chichester, 1991.
14. H. Dugas (Ed.), *Bioinorganic Chemistry*, Springer Verlag, New York, 1996.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) SEMESTER IV

CH4E04 INSTRUMENTAL METHODS OF ANALYSIS (Elective) (4 Credits)

UNIT-I : Optical Methods I

Fundamental laws of spectrophotometry, nephelometry, 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 are), 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 –II : Optical Methods II

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

UNIT-III: Electroanalytical methods:- Basic theory, instrumentation and applications of electrogravimetry, coulometry, polarography, amperometry, biamperometry, cyclic voltametry, chronopotentiometry and stripping analysis.

UNIT-IV : Separation techniques : Liquid-Liquid extraction-distribution laws, use of oxine, dithiazone, high molecular weig ht amines, dithiocarbamates and crown ethers in extraction.

Chromatograpy: Classification, theory, basic instrumentation and use of paper, thin layer, liquid, column, gas, ion-exchange chromatography, Gas chromatography columns, stationary phases and appli cations. Theory and applications of HPLC-LC,LC/MS, LC/MS/MS-Theory and applications of size exclusion, affinity antchiral chromatographic techniques.

UNIT-V : Thermal and Radiochemical Methods (9 Hrs) : Theory

Instrumentation and Applications of (a) Thermogravimetric Analysis (TGA), (b) Differential Thermal Analysis (DTA), (c) Differential Scanning Calorimetry (DSC), (d) Thermometric Titrations, (e) Thermo Mechanical Analysis (TMA) and (f) Dialatometric Analysis(DMA).

UNIT-VI : Environmental analysis : Air pollutants and their fate in the atmosphere, Air quality monitoring and measurement of O_3,CO,SO_2,NO_x,F_2,Cl_3,CFC, hydrocarbon, organosulphur and organotin compounds, Effluent gasses control methods.

Analysis of Water Pollutants: Sources and types of water pollutants as water quality parameters and their determination colour, turbidity, total solids , conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy

metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis.

UNIT-VII : (a) Food Analysis

Moisture, ash, crude protein, fat, crude fiber, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration -common adulterants in food, and their determination for Pesticide analysis in food products. Extraction and estimation of chlorinated pesticides in food products.

Theory of the analysis of milk, butter, other diary items, starch based food products and beverages. Fats and oils -characterization, iodine, bromine and saponification values.

b) Analysis of Body Fluids and Drugs

Clinical chemistry- Composition of blood –collection and preservation of samples, Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphates, hemoglobin, cholesterol, etc.

UNIT – VIII : Enzymes and Immunoassay

General principles, antigen-antibody interactions. Quantitative and qualitative analysis of antigen, Hapten inhibition test, immunodiffusion, immunoelectrophoresis.

Enzyme immunoassay-ELISA and RIA, Fluorescence immunoassay techniques-substrate labeled and delayed enhanced lanthanide fluorescence immunoassay, flow cyctoflourimetry and fluorescence activated cell sorting. Western blotting, Biosensors and chemosensors, amperometeric, potentiometric and colorimetric biosensors.

References :

1. S.M. Khopkar, Basic concepts in Analytical chemistry, wiley Eastern, 2nd edi., 2000.
2. Vogel's Textbook of Quantitative Inorganic Analyses
3. Skoog and West, Principles of Instrumental Analysis
4. Willard, Merrit, Mean and Settle, Instrumental Methods of analysis
5. Official Methods of Analysis of the AOAC.
6. Ayodhya singh, A Textbook of Environmental chemistry, compus books International, New Delhi
7. Sajeev, Moorthy and Kaliappan, Food and Bioprocessing Engineering, Anamaya publishers New Delhi.
8. Wilson.K. and Walker J, Principles and Techniques of practical Biochemistry, Cambridge University press.
9. A.K. De, Environmental chemistry
10. Gary D. Christian, Analytical chemistry, 6th edn, John wiley, 2004

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY – SEMESTER IV

CH4EO5 - COMPUTATIONAL CHEMISTRY (4 credits) (72 h)

Unit I Introduction (9 h): Theory, computation & modeling – Definition of terms; Need of approximate methods in quantum mechanics; Computable Quantities – structure, potential energy surfaces and chemical properties; Cost & Efficiency – relative CPU time, software & hardware; Classification of computational methods.

Unit II Computer simulation methods I (9 h): Introduction – molecular dynamics and Monte Carlo methods, calculation of simple thermodynamic properties - energy, heat capacity, pressure and temperature, phase space, practical aspects of computer simulation, periodic boundary conditions, Monitoring the equilibration, analyzing the results of a simulation, error estimation.

Unit III Computer simulation methods II (9 h): Molecular dynamics (MD) method – molecular dynamics using simple models – MD with continuous potentials, finite difference methods, choosing the time step, setting up and running a MD simulation; Monte Carlo (MC) method - calculating properties by integration, Metropolis method, random number generators, MC simulation of rigid molecules.

UNIT IV ab intio methods in computational chemistry (9h) : Review of Hartree – Fock method for atoms, SCF treatment of polyatomic molecules; Closed shell systems - restricted HF calculations; Open shell systems – ROHF and UHF calculations; The Roothan – Hall equations, Koopmans theorem, HF limit & electron correlation, Introduction to electron correlation (post-HF) methods.

UNIT V Density Functional Methods (9 h): Introduction to density matrices, N-reprentability & V-represetability problems, Hohenberg – Kohn theorems, Kohn-Sham orbitals; Exchange correlation functionals – Thomas-Fermi-Dirac model, Local density approximation, generalised gradient approximation, hybrid functionals; Comparison between DFT and HF methods.

UNIT VI Basis set approximation (9 h): Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, even tempered & well tempered basis sets , contracted basis sets, Pople-style basis sets and their nomenclature, correlation consistent basis sets, basis set truncation error, effect of choice of method/ basis set (model chemistries) on cpu time.

UNIT VII Introduction to Gaussian 03 Program (9h) : Input files – converting a structure from a graphics program – Main features of Gaussian output files – Use of graphics programs like Gaussview, Chemcraft, Molda and Molden in analyzing Gaussian output data - Identification and visualization of normal modes of vibration - Calculation and interpretation molecular orbitals.

UNIT VIII Calculations using G03 Program (9 h): Single point energy calculations; Geometry optimization & Frequency calculations - locating local minima and saddle points on potential energy surfaces, scaling frequencies and zero point energies; Transition state optimizations – characterizing transition states, the normal mode and IRC analyses.

Reference

Text Books

1. C. J. Cramer, *Essentials of computational Chemistry: Theories and models,* John Wiley & Sons 2002.
2. Frank Jensen, *Introduction to Computational Chemistry,* John Wiley & Sons LTD 1999.

3. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.

Further Reading

1. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real-World Problems"*, Wiley-Interscience, 2001.
2. Errol G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2nd edn.*, Springer 2011.
3. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc., 2009.
4. P.W. Atkins & R.S. Friedman, *Molecular quantum mechanics*, 4th Edition, Oxford University Press, 2005.
5. W. Koch, M.C. Holthausen, *"A Chemist's Guide to Density Functional Theory"*, Wiley-VCH Verlag 2000.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER IV

CH4E 06 - MATERIAL SCIENCE (4 credits) (72 h)

UNIT I Introduction to Material Science (9h): Introduction, classification of materials, functional classification, classification based on structure, environmental and other effects, material design and selection;

Mechanical properties – significance and terminology, the tensile test, true stress and true strain, bend test, hardness of materials.

UNIT II Ceramic materials (9h): Definition of ceramics, traditional and new ceramics, structure of ceramics, atomic interactions and types of bonds, phase equilibria in ceramic systems, one component and multi component systems, use of phase diagrams in predicting material behaviour, electrical, magnetic, and optical properties of ceramic materials.

UNIT III Nanomaterials and nanotechnology (9h): Nano materials, nano structures, self assembly, Nano particles - methods of synthesis, sol-gel process, hydrolysis of salts and alkoxides, precipitation, condensation reactions, electrokinetic potential and peptization reactions; Gelation network - xerogels, aerogels, drying of gels; Chemical modification of nano surfaces, applications of sol-gel process, sol-gel coating, porous solids, catalysts, dispersions and powders.

UNIT IV Materials for special purposes – I (9h): Production of ultra pure materials - zone refining, vacuum distillation and electro refining; Ferroelectric and piezoelectric materials - general properties, classification of ferroelectric materials, theory of ferroelectricity, ferroelectric domains, applications, piezoelectric materials and applications; Metallic glasses - preparation, properties and applications.

UNIT V – Materials for special purposes – II (9h): Magnetic materials, ferri and ferro magnetism, metallic magnets, soft, hard & superconducting magnets; Ceramic magnets, low conducting and superconducting magnets; Superconducting materials - metallic and ceramic superconducting materials, theories of superconductivity, Meissner effect; High temperature superconductors - structure and applications.

UNIT VI – Some special polymers (9h): Functional polymers - photoconductive, electroconductive, piezoelectric and light sensitive polymers; Industrial polymers - production, properties, & compounding of industrial polymers; Commodity plastics such as PP, PE, PVC, & PS ; Engineering plastics such as polyacetyl, polyamide (nylon 6 and nylon 66), polyacrylate, polycarbonate, polyester (PET, PBT), polyether ketones; Thermosetting plastics such as PF, UF & MF.

UNIT VII – Composite Materials (9h): Definition and classification of composites, fibres and matrices; Composites with metallic matrices – processing, solid and liquid state processing, deposition;

Ceramic matrix composite materials – processing, mixing & Pressing, liquid state processing, sol-gel processing & vapor deposition technique; Interfaces in composites - mechanical & microstructural characteristics; Applications of composites.

UNIT VIII – Fracture Mechanics (9h): Importance of fracture mechanics, micro structural features of fracture in metals, ceramics, glasses & composites , Weibull statistics for failure, strength analysis; Fatigue, application of fatigue testing - creep, stress rupture & stress behavior, evaluation of creep behavior.

References

1. W.D. Eingery, H.K. Dowen and R.D. Uhlman, *Introduction to Ceramics*, John Wiley.
2. A.G. Guy, *Essentials of Material Science*, McGraw Hill.
3. M.J. Starfield and Shrager, *Introductory Material Science*, McGraw Hill.
4. S.K. Hajra Choudhary, *Material Science and Engineering*, Indian Book Dist. Co., Calcutta.
5. M.W. Barsoum, Fundamentals of Ceramics, McGraw Hill, 1997.
6. M. Tinkham, *Introduction to Superconductivity*, McGraw Hill, 1975.
7. A.V. Narlikar and S.N.Edbote, *Superconductivity and Superconducting Materials*, South Asian Publishers, New Delhi, 1983.
8. S.V. Subramanyan and E.S. Rajagopal, *High Temperature Superconductors*, Wiley Eastern Ltd., 1988.
9. Azaroff and Brophy, *Electronic Processes in Materials*, McGraw Hill, 1985.
10. C.M. Srivastava and C. Srinivasan, Science of Engineering Materials, Wiley Eastern Ltd., 1987.
11. R.J. Young, *Introduction to Polymer Science*, John Wiley and Sons.
12. V.R. Gowriker and Others, *Polymer Science*, Wiley Eastern Ltd.
13. H. Ulrich, *Introduction to Industrial Polymers*, Hansen Publishers, 1982.
14. F.R. Jones, *Handbook of Polymer Fibre Composites*, Longman Scientific and Tech.
15. K.K. Chowla, *Composite Materials*, Springer-Verlag, NY, 1987.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) – SEMESTER IV

CH4E07 INDUSTRIAL CATALYSIS (Elective) (4 credits)

UNIT-I: Introduction to catalysis – General characteristics, Classification,

Description of catalysis- catalytic efficiency, Catalytic performance, activity, turn over number, selectivity, catalyst life, stability, accessibility, mechanical strength, catalytic cycle. Deactivation of catalysts-fouling, cocking, thermal deactivation. Reusability of catalysts, regeneration and recycling, energetic -properties of catalysts.
Experimental aspects in catalyst preparation. Liquid and gas phase reactions, diffusion process, Different types of reactors, tubular reactors, plugged flow, fluid bed reactors etc.

UNIT-II : Homogeneous catalysis - Features of Homogeneous catalysis, various mechanisms and kintetics of acid-base and enzyme catalysis. Catalysts types and mechanisms of the following, Industrially important Homogeneous catalytic processes : Hydrogenation of alkenes, hydroformylation, Monsanto acetic acid synthesis, Wacker oxidation of alkenes, alkene polymersation, surface and supported organometallic catalysis. Asymmetric hydrogenation. Applications of phase transfer catalysis in organic synthesis.

UNIT -III : Heterogeneous catalysis - The nature of heterogeneous catalysts- surface are a and porosity, surface acidic and basic sites, surface metal site, catalytic steps-physical and chemical adsorption, kinetics of chemisorptions, potential energy diagrams, BET and Langmuir adsorption isotherms, mechanisms of Hetrogeneous catalysis - unimolecular and bimolecular surface reactions, Eley –Rideal and Langmuir- Hinshellowood mechanisms.

UNIT-IV : Physical Technique for surface invesugations - Structure of surfaces – Theory and applications of the following techniques for the study of surfaces-Low energy electron diffraction, field electron emission, X-ray and UV photoelectron spectroscopy-ESCA, AES, scanning tunneling microscopy (STM).
X-ray diffraction study, FTIR spectral analysis, UV-Vis spectra ; surface structure analysis, Surface area and pore volume measurements, acid base property studies- Hammett indicator method and temperature programmed adsorption of probe molecules.

UNIT-V : Industrially important heterogeneous catalytic processes – I Hydrogenation : General mechanism and catalyst types of the following processes : Hydrogenation of benzene to cyclohexane, naphthalene to tetraline to decaline, phenol to cyclohexanol, pyridene to piperidine, alkenes to alkanes, alkynes to alkenes, adiponitrile to hexamethylenediamine, nitrobenzene to aniline, n - butaraldehyde to n-butanol, glucose to sorbital, acetone to diacetone alcohol, benzaldehyde to benzyl alcohol, Hydrogenation of Fats and Oils. Isomerization : Mechanism and catalyst types for the conversion of Meta-xylene to para-and ortho-xylenes.
Oxidation : Mechanism and catalyst types for the conversion of propene→ acrolein→ acrylic acid and Methanol→Formaldehyde.

UNIT-VI : Industrially important heterogeneous catalytic process – II
Chemistry and mechanism of ammonia synthesis by Haber-Bosh process, catalyst types and mechanism of the following processes: -

$SO_2 \rightarrow SO_3 \rightarrow H_2SO_4$, $NH_3 \rightarrow NO_2 \rightarrow HNO_3$, $H_2S \rightarrow S$. Shape selective catalysts-zeolites mesoporous materials-various synthesis methods, nanoparticles, super acid catalysts, redox catalyst systems, Supported catalysts - merits, features of supports, role of supports, preparation and structure of supports like silica, alumina, zeolites, carbon, immobilized systems. Electrocatlysis and photocatalysis.

UNIT-VII : Hetrogenerous catalysis in petroleum Refining processes

Catalytic reforming of low octane naphtha to high octane gasoline-chemistry, mechanism and characteristics of typical reforming catalysts. Important catalytic system and mechanisms of Hydrotreating Hydrocraking Isomenization, Oligomrnization, Fluid catalytic cracking.

Synthesis gas- its production and uses. Mechanism and catalyst types for synthesis of methanol, pure CO, H_2 from synthesis gas.

UNIT-VIII: Green chemistry in catalysis

Green aspects of catalysis-application of catalysis in pollution, pollution abatement, methodologies adopted for prevention of pollution through catalytic path, oxidation catalysts, CO oxidation, selective catalytic reduction systems, reduction of nitric oxide, metal nanoparticles in catalysis.

References

1. E.K. Rideal, Concepts in Catalysis, Academic press
2. A. Clark, Theory of adsorption and catalysis, Academic press
3. W.B. Innes, Experimental methods in Catalytic Research Vol.I, Academic press
4. Jens Hagen, Industrial Catalysis-A Practical Approch, Wiley VCH
5. H.F. Rase, Handbook of commercial catalysts , CRC press
6. Ullmann's Encyclopedia of Industrial chemistry
7. Kirk-Othrner Encyclopedia of chemical Technology
8. James clark and D. Macquarrie, Handbook of green chemistry and Technology, Blackwell science, 2002.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CCS PATTERN) SEMESTER IV

CH4EO8 BIOINORGANIC AND ORGANOMETALLIC CHEMISTRY (Elective) (4 Credits)

Unit I: Bioinorganic Chemistry-I (9 h): Coordination sites in biologically important ligands. Thermodynamic and kinetic aspects of stability. Electronic and geometrical structures of metal ions in biology. Role of alkali metal ions in biological systems. Ionophores and passive transport. Sodium pump and active transport.

Unit II: Bioinorganic Chemistry II (9 h): Metallo enzymes and electron carrier metallo proteins. Lewis acid. Role of Zn (II) and Mg (II) containing enzymes. Redox enzymes. Iron enzymes - cytochrome P-450, catalase, peroxidase.

Copper enzymes- Oxidase, superoxide dismutase vitamin B_{12} and Co-enzyme.

Unit III: Bioinorganic Chemistry III (9 h): Transport of oxygen by Heme proteins- hemoglobin and myoglobin. Non heme oxygen carriers, hemerythrin hemocyanin and hemovanadins.

Structure and function of proteins in electron transport process, cytochromes and iron sulphur proteins.

Unit IV: Bioinorganic Chemistry IV (9 h): Bioenergetics and ATP cycle, glucose storage, chlorophyll photosystem I and II. Nitrogenases - Biological nitrogen fixation, other nitrogenases, model systems.

Metal deficiency and diseases, toxic effects of metals, metal complexes used for diagnosis and chemotherapy, Anticancer drugs.

Unit V (9 h): General characteristics of organometallic complexes. Nomenclature, classification, theoretical aspects of 16 and 18 electro rules. Transition metal complexes of H_2, N_2 and Oxygen- Formation structure, bonding and reactions.

Unit VI (9 h): Applications of organometallic compounds in Organic synthesis an catagysis- oxidative addition- reductive elimination and insertion reactions. Substitution reactions in carbonyl complexes - nucleophilic and electrophilic attack on coordinated legands, carbonylation by Collmann's reagent.

Unit VII (9 h): Catalysis, general principles, homogeneous and heterogeneous reactions, catalytic steps.

Homogeneous catalysis: Hydrogenation of alkenes, asymmetric hydrogenation cycloadditions and polymerization of alkynes. Hydroformylation of alkenes, Monsanto acetic acid process, Wacker process.

Unit VIII: Heterogeneous catalysts: Ziegler Natta Catalysis, ammonia synthesis, SO_2 oxidation, zeolite based heterogeneous catalysis catalytic applications involving palladium.

References:

1. S.L. Lippard and J.M. Berry, Principles of Bioinorganic Chemistry, University Science Books, California, 1997.
2. D.E. Fenton, Biocoordination Chemistry, Oxford University Press, Oxford, 1995.
3. Ivam Bertini, Harry B Gray, Stephen. J. Lippard and Joan Selverstone, Valentine, 'Bioinorganic Chemistry', University Science Books, 1994.
4. R.W. Hay, Bioinorganic Chemistry, Ellis Horwoord, 1984.

5. D.F. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chemistry, ELBS, 1990.
6. J.E. Huheey, E.A. Kerter and R.L. Keiter, Inorganic Chemistry, Principles Structure and Reactivity, Pearson, 2001.
7. F.A. Cotton and G. Wilkinson, C.A Murillo and M. Bochmann, Advanced Inorganic Chemistry, John Wiley & Sons, 1999.
8. P. Powell, Principles of Organometallic Chemistry, 2nd Edition, ELBS, 1988.
9. R.C. Mehrothra and A. Singh, Organometallic Chemistry a unified approach, Wiley Eastern, 1991.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) SEMESTER III & IV

CH3PO4 and CH4PO4 – INORGANIC CHEMISTRY PRACTICALS II (4 Credits)

1. Estimation involving quantitative separation of suitable binary mixtures of ions in solution (Cu^{2+}, Nl^{2+}, Zn^{2+}, Fe^{3+}, Ca^{2+}, Mg^{2+}, Ba^{2+} and $Cr_2O_1^{2-}$) by volumetric colorimetric or gravimetric methods only one of the components to be estimated.

2. Colorimetric estimation of Ni, Cu, Fe and Mo after separation from other ions in solution by solvent extraction. (Minimum two expts)

3. Ion- exchange separation and estimation of binary mixtures (Co^{2+} & Nl^{2+}, Zn^{2+} & Mg^{2+} Hardness of water).

4. Preparation of Inorganic Complexes. (5 Nos)

References:

1. Vogel's Text Book of Qualitative Inorganic Analysis.
2. I.M. Kolthoff and E.A. Sanderson, Quantitative Chemical Analysis.
3. D.A. Adams and J.B. Rayner, Advanced Practical Inorganic Chemis try.
4. W.G.Palmer, Experimental Inorganic Chemistry.
5. G. Brauer, Hand book of Preparative Inorganic Chemistry.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (CSS PATTERN) SEMESTER III & IV

CH3PO5, CH4PO5 – ORGANIC CHEMISTRY (4 CREDITS)

UNIT I : Quantitative Organic Analysis

Estimation of equivalent weight of acids by Silver Salt method, Estimation of nitrogen by Kjeldahl method, Determination of Acid value, iodine value and saponification value of oils and fats (at least one each), Estimation of reducing sugars, Estimation of amino group, phenolic group and esters. Colourimetric estimations: Vitamins (Ascorbic acid), Drugs – sulpha drug (Sulpha diazine, sulphaguanidine), Antibiotics – Pencillin, Stroptomycin.

References

1. B.S. Furnis, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry* , ELBS/Longman, 1989.
2. Beebet, *Pharmacuetical Analysi*.

UNIT II : Extraction of Natural products and purification by column chromatography and TLC – Caffeine from Tea waste, Chlorophill Steroids, Flavonoid (Soxhlet extraction), citral from lemon glass (steam distillation). Casein from milk.

UNIT III : Practical application of PC and TLC, Preparation of TLC plates, Activation, Identification of the following classes of compounds using

one- and two-dimensional techniques. Identification by using spray reagents and co-chromatography by authentic samples and also from Rf values.

Food additives and Dyes, Artificial sweeteners: Saccharine, cyclamates, Dulcin. Flavour adulterants – piperonal, Benzalacetate, ethyl acetate antioxidants: Butylated hydroxytoluene (BHT) Butylated hydroxy anisole (BHA), Hydroquinone.

Food colours: Permitted – Amaranth, Erythrosine, Tatrazine, susnet yellow, Fast green, Brilliant Blue, Nonpermitted colours : Auramine, Congo red, Malachite green, Metanil yellow, Orange II, Sudan II, Congo red.

Amino acids (Protein hydrolysates), Sugars, Terpinoids, Alkaloids, Flavonoids, Steroids.

Pesticides and herbicides: Oragonochlorine pesticides organo phosphates and carbamate pesticides, Herbicides.

Plant growth stimulants: Indolacetic acid.

References

1. E. Hoftmann, *Chromatography*, non Nostrand Reinhold Company, New York, 1975.

2. J. Sherma and G. Zwig, *TLC and LC analysis of pesticides of international importance*, Vol. VI & VII, Academic Press.

3. H. Wagner, S. Bladt, E.M. Zgainsti – Tram, Th. A. Scott., *Plant Drug Analysis*, Springer-Verlag, Tokyo, 1984.

UNIVERSITY OF CALICUT

M.Sc. CHEMISTRY (III & IV Semesters)

CH3PO6, CH4PO6 – PHYSICAL CHEMISTRY PRACTICAL II

(4 credits) (36 LS)

UNIT I : Chemical Kinetics (4 experiments)

1. Determination of specific reaction rate of acid hydrolysis of an ester (methyl acetate or ethyl acetate) and concentration of the given acids.
2. Determination of Arrhenius parameters of acid hydrolysis of an ester.
3. Determination of specific reaction rate of saponification of ethyl acetate.
4. Iodination of acetone in acid medium – Determination of order of reaction with respect of iodine and acetone.

UNIT II Adsorption (3 experiments)

1. Verification of Langmuir adsorption isotherm – charcoal-acetic acid system.

   Determination of the concentration of a given acetic acid solution using the isotherm
2. Verification of Langmuir adsorption isothem – charcoal-oxalic acid system.

   Determination of the concentration of a given acetic acid solution using the isothem.
3. Determination of surface area of adsorbent.

UNIT III Phase Equilibria (2 experiments)

1. (a) Determination of phase diagram of a ternary liquid system (e .g., chloroform – acetic acid – water – Benzene – acetic acid – water)

   (b) Determination of the composition of a binary liquid mixture (e.g., chloroform-acetic acid, benzene-acetic acid)

2. (a) Determination of mutual miscibility curve of a binary li quid system (e.g., phenol – water) and critical solution temperature (CST).

   (b) Effect of impurities (e.g, NaCl, KCl, succinic acid, salicylic acid) on the CST of water-phenol system)

   (c) Effect of a given impurity (e.g., KCl) on the CST of water -phenol system and determination of the concentration of the given solution of KCl.

UNIT IV Cryoscopy – Beckman thermometer method (3 experiments)

1. Determination of cyroscopic constant of a liquid (water, benzene)

2. Determination of molecular mass of a soute (urea, glucose, cane sugar, mannitol) by studying the depression in freezing point of a liquid solvent (water, benzene)

3. Determination of Van't Hoff factor and percentage of dissociation of NaCl.

4. Study of the reaction $2Kl + Hgl_2 \rightarrow K_2Hgl_4$ and determination of the concentration of the given Kl solution.

UNIT V Polarimetry (3 experiments)

1. Determination of specific and molar optical rotations of glucose, fructose and sucrose.

2. Determination of specific rate of inversion of cane sugar in presence of HCl.

3. Determination of concentration of HCl

UNIT VI Spectrophotometry (3 experiments)

1. Determination of equilibrium constants of acid -base indicators.

2. Simultaneous of determination Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$

3. Investigation of complex formation between Fe (III) and thiocyanate.

Reference

1. A. Finlay and J.A. Kitchener, *Practical Physical Chemistry,* Longman.
2. F. Daniels and J.H. Mathews, *Experimental Physical Chemistry,* Longman.
3. A.H. James, *Practical Physical Chemistry*, J.A. Churchil Ltd., 1961.
4. H.H. Willard, L.L. Merit and J.A. Dean, *Instrumental Methods of Analysis,* 4th Education, Affiliated East-West Press Pvt. Ltd., 1965.
5. D.P. Shoemaker and C.W. Garland, *Experimental Physical Chemistry,* McGraw Hill.
6. J.B. Yadav, *Advanced Practical Physical Chemistry, Goel Publications,* 1989.

SECTION B

UNIT VII Computer Applications in Chemistry(8 experiments)

(The experiment consist of writing a computer programme in C language for a problem of chemical interest and its execution using a computer. The student shall generate a hard copy of the programme and the results using a printer for submission)

1. Calculation of dipole moments of disubsituted benzenes.
2. Calculation of delocalization energy.
3. Determination of lattice energy of ionic crystals musing Born Lande equation.
4. Determination of solubility of sparingly soluble salts.
5. Determination of half life & average life of a radioactive element.
6. Determination of molecular weight of an organic compound.
7. Determination of first ten energy levels of i) an electron ii) a helium atom iii) carbon 60 and iv) a particle of mass μg confined in a one-dimensional box of length 100nm and comparison of energy spacing of these systems.
8. Comparison of the translational quantum numbe rs of i) an electron ii) helium atom iii) carobon-60 and iv) a 1-μg particle confined in a one-dimensional box of length 100nm at room temperature ($E = n^2h^2/8ma^2 = kT/2$).
9. Determination of Arrhenius parameters of acid hydrolysis of methyl acetate by the method of least squares by writing a C programme (Necessary kinetic data are provided).
10. Verification of Langmuir and Freundlisch adsorption isothems by the method of least square by writing a C programme and determination of adsorption parameters. (Necessary adsorption data are provided)

Reference

1. K.V. Raman, *Computer in Chemistry,* Tata McGraw Hill, 1993.
2. E. Balaguruswamy, *Programming in* C. Macmillan India Ltd., 1991.
3. Michael, A. Vine, *C. Programming for the Absolute Beginner,* Thompson Course Technology, 2007.
4. Dan Gookin, *C. Programming,* John Wiley and Sons, 2004.
5. K.B. Wiberg, *Computer Programming for Chemists,* Benjamin Inc, NY, 1965.
6. P.Lykose, *Personal Computers in Chemistry,* John Wiley and sons, NY, 1981.

QUESTION PAPER

1. Each student is required to answer two questions, one based on one or more units in Section A (60 marks) and the other from Section B (20 marks)

2. Each student in a batch shall be given separate questions.