BRANCH VA

M. Sc.
APPLIED CHEMISTRY

FOREWORD

I feel highly privileged in presenting the revised curricula and syllabi of Branch VA M.Sc. Applied Chemistry for favour of approval by the Faculty and Academic Council of the University.

As per Mahatma Gandhi University PG Programme Regulations for Credit Semester System 2011(MGU-CSS-PG) it has been decided to introduce the Credit Semester System for all the PG courses which are being offered by the affiliated colleges/institutions of the University with effect from the academic year 2012-2013 admission onwards. The PG Board of Studies in Chemistry was entrusted with the duty of preparing the revised curricula and syllabi for all the five M.Sc. Programmes in Chemistry currently approved by the University and offered in the affiliated colleges.

The BOS prepared draft proposals of revised curricula and syllabi for all the M.Sc. courses in Chemistry in conformity with the broad guidelines issued by the University to suit the Credit Semester System. The draft curricula and syllabi for all the five M.Sc. Programmes were discussed in a very effective manner with active participation of Resource Persons and Teacher Representatives from all the colleges in a three-day workshop. The workshop was a grand success and the BOS could incorporate many of the suggestions while finalizing the proposal of the Restructured Curricula and Syllabi.

The BOS feel that appreciable updating could be done in keeping with the current developments and trends in chemistry education. The task of preparing the Curricula and Syllabi and bringing it out in the present form for all the five M.Sc. courses was not a simple task but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS. I would like to express my sincere thanks to all my fellow members of the BOS for all their whole hearted time-bound help, cooperation and encouragement. It has been a pleasure for me to work with them. I am also thankful to all Resource Persons and Teacher Representatives of the colleges for their active participation and useful suggestions during the three-day workshop.

Prof. (Dr.) P. K. Radhakrishnan
Chairman, PG Board of Studies in Chemistry

PG Board of Studies in Chemistry

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	Code	Course	Hours /Week	Total Hours	Credit
Semester 1	AP1C01	Organometallics and Nuclear Chemistry	4	72	4
	AP1C02	Structural and Molecular Organic Chemistry	4	72	4
	AP1C03	Quantum Chemistry and Group Theory	4	72	4
	AP1C04	Classical and Statistical Thermodynamics	3	54	3
	AP2P01	Inorganic Chemistry Practical	3	54	Evaluation at the end of second
	AP2P02	Organic Chemistry Practical	3	54	
	AP2P03	Physical Chemistry Practical	4	72	
		Total	**25**	**450**	**15**
Semester 2	AP2C05	Coordination Chemistry	4	72	4
	AP2C06	Organic Reaction Mechanisms	4	72	4
	AP2C07	Chemical Bonding and Computational Chemistry	4	72	4
	AP2C08	Molecular Spectroscopy	3	54	3
	AP2P01	Inorganic Chemistry Practical	3	54	3
	AP2P02	Organic Chemistry Practical	3	54	3
	AP2P03	Physical Chemistry Practical	4	72	3
		Total	**25**	**450**	**24**
Semester 3	AP3C09	Advanced Synthetic Organic Chemistry	4	72	4
	AP3C10	Chemistry and Biochemistry of Fatty Acids	4	72	4
	AP3C11	Essential Oils and Aromatics	4	72	4
	AP3C12	Physical Methods in Chemistry	3	54	4
	AP4P04	Industrial Oil and Fat Products Practical	4	72	Evaluation at the end of fourth semester
	AP4P05	Essential Oils and Aromatics	3	54	
	AP4P06	Fixed Oils and Fats Practical	4	72	
		Total	**25**	**450**	**15**
Semester 4		Elective 1	5	90	4
		Elective 2	5	90	4
		Elective 3	5	90	4
	AP4P04	Industrial Oil and Fat Products Practical	3	54	3
	AP4P05	Essential Oils and Aromatics	3	54	3
	AP4P06	Fixed Oils and Fats Practical	4	72	3
	AP4D01	Project			3
	AP4V01	Viva			2
		Total	**25**	**450**	**26**
Grand Total					**80**

SEMESTER 1

AP1C01 ORGANOMETALLICS AND NUCLEAR CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hours)

1.1 Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

1.2 Complexes with cyclic pi donors-metallocenes and cyclic arene complexes-structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.

1.3 Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons.

Unit 2: Reactions of Organometallic Compounds (9 Hrs)

2.1 Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

2.2 Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.

2.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Unit 3: Catalysis by Organometallic Compounds (9 Hrs)

3.1 Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.

3.2 Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer-Tropsch reaction(synthesis of gasoline).

3.3 Hydroformylation of olefins using cobalt or rhodium catalyst.

3.4 Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts.

3.5 Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis.

3.6 Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("Platinum Pop"). Palladium catalysed oxidation of ethylene-the Wacker process.

Unit 4: Organometallic Polymers (9 Hrs)

4.1 Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Unit 5: Bioinorganic Compounds (18 Hrs)

5.1 Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+, ATP and ADP. Photosynthesis-chlorophyll a, PS I and PS II. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.

5.2 Oxygen carriers and oxygen transport proteins-haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems-ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes-CarboxypeptidaseA-structure and functions. Nitrogen Fixation-nitrogenase, vitamin B_{12} and the vitamin B_{12} coenzymes.

5.3 Metals in medicine-therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals(Cd, Hg, Cr and Pb).

Unit 6: Nuclear Chemistry (9 Hrs)

6.1 Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations. Positron annihilation and autoradiography. Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.

6.2 Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.

6.3 Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.

6.4 Applications of radio isotopes in industry, medicine, audiography, radiopharmacology, radiation safety precaution, nuclear waste disposal. Radiation chemistry of water and aqueous solutions.

6.5. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

References

01. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers,1993.

02. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999.

03. K.F. Purcell, J. C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

04. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988.

05. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.

06. B.D. Guptha, A.J. Elias, Basic Organometallic Chemistry, Universities Press, 2010.

07. R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1984.

08. H.J. Amikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1982.

09. S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

AP1C02 STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Basic Concepts in Organic Chemistry (18 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridisation, MO picture, inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

1.2 The formalism of curved arrow mechanisms. Practicing of line diagram drawing.

1.3 Concept of aromaticity: delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems - annulenes. NMR as a tool for aromaticity. Anti-and homo-aromatic systems - Fullerenes, Carbon nanotubes and Graphene.

1.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. SN1, SNAr, SRN1 and Benzyne mechanisms.

Unit 2: Physical Organic Chemistry and Photochemistry (18 Hrs)

2.1 Energy profiles. Kinetic versus thermodynamic control of product formation, Hammond postulate, kinetic isotope effects with examples, Hammet equation, Taft equation.

2.2 Catalysis by acids and bases and nucleophiles with examples from acetal, cyanhydrin and ester formation and hydrolysis reactions –A_{AC}^2, A_{AC}^1, A_{AL}^1, B_{AC}^2 and B_{AL}^1 mechanisms, solvent effect. Linear free energy relationship. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Hard and soft acids and bases - HSAB principle and its applications.

2.3 Photoreactions of carbonyl compounds: enes, dienes, dienones and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi reaction. Barton, Di-π-methane and photo Fries rearrangements. Photochemistry of nitro and azo groups.

Unit 3: Stereochemistry of Organic Compounds (18 Hrs)

3.1 Introduction to molecular symmetry and chirality: examples from common objects to molecules. Axis, plane, center, alternating axis of symmetry.

3.2 Center of chirality: molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and Cn, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro, threo nomenclature.

3.3 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidenecycloalkanes.

3.4 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.

3.5 Stereoisomerism: definition based on symmetry and energy criteria, configuration and conformational stereoisomers.

3.6 Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

Unit 4: Conformational Analysis (18 Hrs)

4.1 Conformational descriptors - factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Fused and bridged bicyclic systems. Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination-Saytzeff and Hofmann eliminations), substitution and oxidation of 2^0 alcohols. Chemical consequence of conformational equilibrium -Curtin Hammett principle.

References

01. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.

02. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer, 2007.

03. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

04. T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2nd Edn., Harper & Row, 1981.

05. N.S. Isaacs, Physical Organic Chemistry, ELBS/Longman, 1987.

06. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 3rd Edn., New Age Pub., 2010.

07. D.G. Morris, Stereochemistry, RSC, 2001.

08. E.L. Eliel and S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 1994.

09. N.J. Turro, V. Ramamurthy, J.C. Scaiano, Principles of Molecular Photochemistry: An Introduction, University Science books, 2009.

10. N.J. Turro, Modern Molecular Photochemistry, Benjamin Cummings, 1978.

11. K.K.R. Mukherjee, Fundamentals of Photochemistry, New Age Pub., 1978.

AP1C03 QUANTUM CHEMISTRY AND GROUP THEORY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Postulates of Quantum Mechanics (9 Hrs)

1.1 State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions.

1.2 Operator postulate: operator algebra, linear and nonlinear operators, Laplacian operator, commuting and noncommuting operators, Hermitian operators and their properties, eigen functions and eigen values of an operator.

1.3 Eigen value postulate: eigen value equation, eigen functions of commuting operators.

1.4 Expectation value postulate.

1.5 Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.

Unit 2: Application to Exactly Solvable Model Problems (18 Hrs)

2.1 Translational motion: free particle in one-dimension, particle in a one-dimensional box with infinite potential walls, particle in a one-dimensional box with finite potential walls-tunneling, particle in a three dimensional box-separation of variables, degeneracy.

2.2 Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation(solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.

2.3 Rotational motion: co-ordinate systems, cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates-particle on a ring, the phi equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)-polar diagrams of spherical harmonics.

2.4 Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (L_x, L_y, L_z and L^2)-commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Ladder operator method for angular momentum. Space quantization.

Unit 3: Quantum Mechanics of Hydrogen-like Atoms (9 Hrs)

3.1 Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables-R, theta and phi equations and their solutions,

wave functions and energies of hydrogen-like atoms. Orbitals-radial functions, radial distribution functions, angular functions and their plots.

3.2 The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin-Stern Gerlach experiment. Spin orbitals-construction of spin orbitals from orbitals and spin functions.

Unit 4: Symmetry and Groups (9 Hrs)

4.1 Symmetry elements, symmetry operations, point groups and their symbols, sub groups, classes, abelian and cyclic groups, group multiplication tables-classes in a group and similarity transformation.

4.2 Symmetry in crystals-32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis. Glide planes. Space groups-determination of space group symbols of triclinic and monoclinic systems.

Unit 5: Theory of Molecular Symmetry (18 Hrs)

5.1 Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic orbitals as basis, representation generated by cartesian coordinates positioned on the atoms of a molecule (H_2O and SO_2 as examples).

5.2 Reducible and irreducible representations-construction of irreducible representation by standard reduction formula. Statement of Great Orthogonality Theorem (GOT). Properties of irreducible representations. Construction of irreducible representation using GOT-construction of character tables for C_{2v}, C_{2h}, C_{3v} and C_{4v}. Direct product of representations.

5.3 Molecular dissymmetry and optical activity.

Unit 6: Application of Group Theory in Spectroscopy (9 Hrs)

6.1 Applications in vibrational spectra: symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Complementary character of IR and Raman spectra-determination of the number of active IR and Raman lines.

6.2 Application in electronic spectra: electronic spectra of diatomic molecules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, types of electronic transitions, Fortrat diagram, dissociation and pre dissociation, calculation of heat of dissociation.

References

01. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.

02. P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press, 2005.

03. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

04. J.P. Lowe, K Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006.

05. R. Anatharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2001.

06. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.

07. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006.

08. H. Metiu, Physical Chemistry:Quantum Mechanics, Taylor & Francis, 2006.

09. L. Pauling, E.B. Wilson, Introduction to Quantum Mechanics, McGraw-Hill, 1935.

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

11. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.

12. L.H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill,1969

13. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.

14. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.

15. S.F.A. Kettle, Symmetry and Structure: Readable Group Theory for Chemists, 3rd Edn**.,** Wiley, 2007.

16. A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edn., Wiley, 2000.

17. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010

AP1C04 CLASSICAL AND STATISTICAL THERMODYNAMICS

Credit: 3 **Contact Lecture Hours- 54**

Unit 1: Classical Thermodynamics (27 Hrs)

1.01 Entropy, dependence of entropy on variables of a system (S,T and V; S,T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.

1.02 Free energy, Maxwell relations and significance, temperature dependence of free energy - Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.

1.03 Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

1.04 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.

1.05 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions-free energy, enthalpy, entropy and volume. Determination of excess enthalpy and volume.

1.06 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- vant Hoff reaction isochore and isotherm.

1.07 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

1.08 Three component systems-graphical representation. Solid-liquid equilibria-ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria-one pair of partially miscible liquids, two pairs of partially miscible liquids, three pairs of partially miscible liquids.

1.09 Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, the Onsager reciprocal relations. Thermal osmosis. Thermoelectric phenomena.

1.10 Bioenergetics: coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

Unit 2: Statistical Thermodynamics (27 Hrs)

2.1 Permutation, probability, apriori and thermodynamic probability, Stirlings approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function-translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength.

2.2 Calculation of thermodynamic functions and equilibrium constants, statistical interpretation of work and heat, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual

entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

2.3 Need for quantum statistics, Bose-Einstein statistics: Bose-Einstein distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi-Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics.

2.4 Heat capacity of solids- the vibrational properties of solids, Einsteins theory and its limitations, Debye theory and its limitations.

References

01. R.P. Rastogi, R.R. Misra, An Introduction to Chemical Thermodynamics, Vikas Publishing House, 1996.

02. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.

03. M.C. Gupta, Statistical Thermodynamics, New age international, 2007.

04. M.W. Zemansky, R.H. Dittman, Heat and Thermodynamics, Tata McGraw Hill, 1981.

05. P.W. Atkins, Physical Chemistry, ELBS, 1994.

06. K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4th Edn., Houghton Mifflin, 2003.

07. L.K. Nash, Elements of Classical and Statistical Mechanics, 2nd Edn., Addison Wesley, 1972.

08. D.A. McQuarrie, J.D. Simon, Physiacl chemistry: A Molecular Approach, University Science Books,1997

09. C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002.

10. R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper's Biochemistry, Tata McGraw Hill,1999.

11. I. Tinoco, K. Sauer, J.C. Wang, J.D. Puglisi, Physical Chemistry: Principles and Applications in Biological Science, Prentice Hall,2002

12. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, 1975.

13. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971.

SEMESTER 2

AP2C05 COORDINATION CHEMISTRY

Credits: 4 **Contact Lecture Hours: 72**

Unit 1: Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. Sigma and pi bonding ligands such as CO, NO, CN^-, R_3P, and Ar_3P. Stability of complexes, thermodynamic aspects of complex formation-Irving William order of stability, chelate effect.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and triagonal bipyramidal fields, LFSE, *Dq* values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory-M.O energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for pi-bonding.

Unit 2: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

2.1 Electronic Spectra of complexes-Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.

2.2 Interpretation of electronic spectra of complexes-Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of *Dq*, *B* and β (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.

2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism-Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism-inter and intramolecular interaction. Anomalous magnetic moments.

2.4 Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.

Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, *trans* effect-theory and applications.

3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).

3.3 Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism.

Unit 4: Stereochemistry of Coordination Compounds (9 Hrs)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds,

4.2 Linkage isomerism-electronic and steric factors affecting linkage isomerism. Symbiosis-hard and soft ligands, Prussian blue and related structures, Macrocycles-crown ethers.

Unit 5: Coordination Chemistry of Lanthanides and Actinides (9 Hrs)

5.1 General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents.

5.2 General characteristics of actinides-difference between *4f* and *5f* orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

References

01. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.

02. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.

03. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.

04. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.

05. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.

06. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

07. B.N. Figgis, M.A. Hitchman, Ligand field Theory and its Applications, Wiley-India, 2010.

08. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008

09. A.B.P. Lever, Inorganic Electronic Spectroscopy, 2nd Edn., Elsevier, 1984.

10. S. Cotton, Lanthanide and Actinide Chemistry, John Wiley & Sons, 2007.

11. T. Moeller, International Review of Science: Inorganic Chemistry, Series I, Vol VII, Butterworth, 1972.

AP2C06 ORGANIC REACTION MECHANISM

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Review of Organic Reaction Mechanisms (9 Hrs)

1.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (SN_1, SN_2, SN_i, SE_1, SE_2, addition-elimination and elimination-addition sequences), elimination (E_1 and E_2) and addition reactions (regioselectivity: Markovnikov's addition-carbocation mechanism, anti-Markovnikov's addition-radical mechanism). Elimination vs substitution.

1.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution(SN_2 and SN_1) and elimination (E_1 and E_2) reactions.

Unit 2: Chemistry of Carbanions (9 Hrs)

2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates- lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates.

2.2 Nucleophilic additions to carbonyls groups. Named reactions under carbanion chemistry-mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.

2.3 Ylids: chemistry of phosphorous and sulphur ylids - Wittig and related reactions, Peterson olefination.

Unit 3: Chemistry of Carbocations (9 Hrs)

3.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.

3.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.

3.3 C-C bond formation involving carbocations: oxymercuration, halolactonisation.

Unit 4: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

4.1 Structure of carbenes (singlet and triplet), generation of carbenes, addition and insertion reactions.

4.2 Rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

4.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.

4.4 Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

4.5 Arynes: generation, structure, stability and reactions. Orientation effect-amination of haloarenes.

Unit 5: Radical Reactions (9 Hrs)

5.1 Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements-Hydroperoxide: formation, rearrangement and reactions. Autooxidation.

5.2 Named reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Unit 6: Chemistry of Carbonyl Compounds (9 Hrs)

6.1 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolf-Kishner), addition (addition of cyanide, ammonia, alcohol) reactions, Cannizzaro reaction, addition of Grignard reagent. Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition-Michael addition, Mannich reaction, Robinson annulation.

Unit 7: Concerted reactions (18 Hrs)

7.1 Classification: electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions. Woodward Hoffmann rules - frontier orbital and orbital symmetry correlation approaches - PMO method.

7.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (with stereochemical aspects), dipolar cycloaddition(introductory).

7.3 Unimolecular pyrolytic elimnination reactions: cheletropic elimination, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

7.4 Problems based on the above topics.

References

01. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

02. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5th Edn., Springer, 2007.

03. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.

04. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edn., Wiley, 2007.

05. A. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.

06. S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005.

07. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, Organic Chemistry, 7th Edn., Pearson, 2011.

08. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

AP2C07 CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 72**

Unit 1: Approximate Methods in Quantum Mechanics (18 Hrs)

1.1 Many-body problem and the need of approximation methods, independent particle model. Variation method, variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box and using the trial function e^{-ar} for the hydrogen atom, variation treatment for the ground state of helium atom.

1.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

1.3 Hartree Self-Consistent Field method. Spin orbitals for many electron atoms-symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Unit 2: Chemical Bonding (18 Hrs)

2.1 Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.

2.2 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, N_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order. Correlation diagrams, non-crossing rule. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.

2.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond orders and free valency.

Unit 3: Applications of Group Theory in Chemical Bonding (9 Hrs)

3.1 Application in quantum mechanics, transition moment integral, vanishing of integrals.

3.2 Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{2h}, C_3, C_{3v} and D_{3h}. Jahn-Teller effect. Woodward Hoffmann rules-correlation diagram.

Unit 4: Computational Chemistry (18 Hrs)

(The units 4 and 5 have been designed to expose the students to the field of computational chemistry, which has emerged as a powerful tool in chemistry capable of supplementing and complementing experimental research. The quantities which can be calculated using computational methods, how to prepare the input to get these results and the different methods that are widely used to arrive at the results are introduced here. Detailed mathematical derivations are not expected. Though computer simulations form an important part of computational chemistry, they are not covered in this syllabus.)

4.1 Introduction: computational chemistry as a tool and its scope.

4.2 Potential energy surface: stationary point, transition state or saddle point, local and global minima.

4.3 Molecular mechanics methods: force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions. Mathematical expressions. Parameterisation from experiments or quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.

4.4 Ab initio methods: A review of Hartee-Fock method. Basis set approximation. Slater and Gaussian functions. Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

4.5 Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods-variational method, basic principles of Configuration Inetraction(CI). Perturbational methods-basic principles of Møller Plesset Perturbation Theory.

4.6 General introduction to semiempirical methods: basic principles and terminology.

4.7 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).

4.8 Model Chemistry-notation, effect on calculation time (cost).

4.9 Comparison of molecular mechanics, ab initio, semiempirical and DFT methods.

Unit 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input-cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS / Firefly input file. GAMESS / Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

5.2 Identifying a successful GAMESS/ Firefly calculation-locating local minima and saddle points, characterizing transition states, calculation of ionization energies, Koopmans' theorem, electron affinities and atomic charges.

5.3 Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.

References

01. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.

02. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

03. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.

04. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.

05. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.

06. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning Pvt. Ltd., 2010

07. E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.

08. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.

09. F. Jensen, Introduction to computational chemistry, 2nd Edn., John Wiley & Sons, 2007.

10. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn., Longman, 2001.

11. J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011.

12. K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008.

13. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008.

14. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.

15. D.C. Young, Computational Chemistry:A Practical Guide for Applying Techniques to Real-World Problems, John Wiley & Sons, 2001.

Softwares

Molecular Mechanics:

1. **Arguslab** available from www.arguslab.com/
2. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

1. **Firefly / PC GAMESS** available from http://classic.chem.msu.su/gran/gamess/
2. **WINGAMESS** available from http://www.msg.ameslab.gov/gamess/

Graphical User Interface (GUI):

1. **Gabedit** available from http://gabedit.sourceforge.net/
2. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
3. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

AP2C08 MOLECULAR SPECTROSCOPY

Credit: 3 **Contact Lecture Hours: 54**

Unit 1: Foundations of Spectroscopic Techniques (27 Hrs)

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width, contributing factors, Doppler broadening, Lamb dip spectrum, Born Oppenheimer approximation, energy dissipation from excited states (radiative and non radiative processes), relaxation time.

1.2 Microwave spectroscopy: principal moments of inertia and classification (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max} , effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.

1.3 Infrared spectroscopy: Morse potential energy diagram, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, disadvantages of dispersive IR, introduction to FT spectroscopy, FTIR.

1.4 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.

1.5 Electronic spectroscopy: term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model, different types of lasers-solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

Unit 2: Resonance Spectroscopy (27 Hrs)

2.1 NMR spectroscopy : interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.

2.2 FTNMR, second order effects on spectra, spin systems (AB, AB_2), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR, natural abundance, sensitivity, ^{13}C

chemical shift and structure correlation, introduction to solid state NMR, magic angle spinning.

2.3 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values (g_{II} and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

2.4 An elementary study of NQR spectroscopy.

2.5 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes, MB spectra of Fe(II) and Fe(III) cyanides.

References

01. C.N. Banwell, E.M.McCash, Fundamentals of molecular spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

02. G. Aruldhas, Molecular structure and spectroscopy, Prentice Hall of India, 2001.

03. P.W. Atkins, Physical Chemistry, ELBS,1994

04. R.S. Drago, Physical Methods in Inorganic Chemistry, Van Nonstrand Reinhold, 1965.

05. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.

06. K.J. Laidler, J.H. Meiser, Physical Chemistry, 2nd Edn., CBS, 1999.

07. W. Kemp, NMR in chemistry-A multinuclear introduction, McMillan, 1986.

08. H. Kaur, Spectroscopy, 6th Edn., Pragati Prakashan, 2011.

09. H. Gunther, NMR spectroscopy, Wiley, 1995.

10. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books,1997.

11. D.N. Sathyanarayan, Electronic Absorption Spectroscopy and Related Techniques, Universities Press, 2001.

12. D.N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2007

13. D.N. Sathyanarayana, Introduction To Magnetic Resonance Spectroscopy ESR,NMR,NQR, IK International, 2009.

SEMESTERS 1 AND 2

AP2P01 INORGANIC CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li. Anions which need elimination not to be given. Minimum eight mixtures to be given.

PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions.

PART III

Preparation and characterization complexes using IR, NMR and electronic spectra.

(a) Tris (thiourea)copper(I) complex

(b) Potassium tris (oxalate) aluminate (III).

(c) Hexammine cobalt (III) chloride.

(d) Tetrammine copper (II) sulphate.

(e) Schiff base complexes of various divalent metal ions.

References

01. A.I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.

02. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman,1966.

03. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., Mc Millian, 1968.

04. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.

AP2P02 ORGANIC CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

PART II

1. Separation of Organic binary mixtures by chemical/solvent separation methods
2. Separation of organic mixtures by TLC
3. Separation/ purification of organic mixtures by column chromatography

PART III

Drawing the structures of organic molecules and reaction schemes by ChemDraw, Symyx Draw and Chemsketch. Draw the structures and generate the IR and NMR spectra of the substrates and products in the following reactions:

1. Cycloaddition of diene and dienophile (Diels-Alder reaction)
2. Oxidation of primary alcohol to aldehyde and then to acid
3. Benzoin condensation
4. Esterification of simple carboxylic acids
5. Aldol condensation

References

01. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

03. F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

04. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

AP2P03 PHYSICAL CHEMISTRY PRACTICAL

Credit: 3 **Contact Lab Hours: 72+72 =144**

(One question each from both parts A and B will be asked for the examination)

Part A

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.
2. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by
   a) Capillary rise method
   b) Drop number method
   c) Drop weight method
2. Determination of parachor values.
3. Determination of the composition of two liquids by surface tension measurements

Part B

Computational chemistry experiments

V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

References

01. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

02. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.

03. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.

04. GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html

SEMESTER 3

AP3C09 ADVANCED SYNTHETIC ORGANIC CHEMISTRY

Credit : 4 **Contact Lecture Hours: 72**

Unit 1: Organic Synthesis via Oxidation and Reduction (9 Hrs)

1.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium and DMSO based reagents). (b) alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation.(c) alkenes to diols (Manganese and Osmium based), Prevost reaction and Woodward modification, (d) alkenes to carbonyls with bond cleavage (Manganese and lead based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium/chromium based allylic oxidation) (f) ketones to esters/lactones (Baeyer-Villiger).

Unit 2: Modern Synthetic Methods and Reagents (9 Hrs)

2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Noyori reaction. Brook rearrangement, Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Suzuki-Miyaura, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions, Wohl-Ziegler reaction. Reagents such as: NBS, DDQ, DCC, Gilmann reagent.

2.2 Introduction to multicomponent reactions, Click reactions.

Unit 3: Stereoselective Transformations (9 Hrs)

3.1 Assymmetric induction, chiral auxiliaries and chiral pool.
3.2 Enatioselective catalytic hydrogenation developed by Noyori and Knowels.
3.3 Assymetric aldol condensation pioneered by Evans.
3.4 Assymmetric Diels Alder reactions.
3.5 Assymmetric epoxidation using Jacobsen’s catalyst.

Unit 4: Construction of Carbocyclic and Heterocyclic Ring Systems (9 Hrs)

4.1 Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes. ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, Mitsunobu reaction, cation-olefin cyclization and radical-olefin cyclization.

4.2 Inter-conversion of ring systems (contraction and expansion), Demjenov reaction, Reformatsky reaction. Construction of macrocyclic rings, ring closing metathesis.

4.3 Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more hetero atom like N, S or O: pyrrole, furan, thiophene, imidazole, thiazole and oxazole.

Unit 5: Molecular Recognition and Supramolecular Chemistry (9 Hrs)

5.1 Concept of molecular recognition, host-guest complex formation, forces involved in molecular recognition.

5.2 Molecular receptors: Cyclodextrins, Crown ethers, Cryptands, Spherands, Tweezers, Carcerands, Cyclophanes, Calixarenes, Carbon nanocapsules.

5.3 Importance of molecular recognition in biological systems like DNA and protein, Controlled release phenomena.

5.4 Applications of supramolecular complexes in medicine and perfumery industries.

Unit 6: Chemistry of Natural products and Biomolecules (9 Hrs)

6.1 Basic aspects of structure and classification of carbohydrates, alkaloids, steroids, plant pigments, vitamins, amino acids, proteins and nucleic acids.

6.2 Methods for primary structure determination of peptides, proteins and nucleic acids. Replication of DNA. Flow of genetic information. Protein biosynthesis. Transcription and translation. Genetic code. Regulation of gene expression. DNA sequencing. The Human Genome Project. DNA profiling and the Polymerase Chain Reaction (PCR).

Unit 7: Reterosynthetic Analysis (9 Hrs)

7.1 Basic principles and terminology of reterosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections.

7.2 Amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Enantioselective synthesis of Corey lactone, Longifolene and luciferin. Umpolung equivalence, Peterson olefination, enolate formation, Ireland method.

Unit 8: Green Alternatives of Organic Synthesis (9 Hrs)

8.1 Principles of Green Chemistry, Basic concepts, Atom Economy, Principles of Green Organic Synthesis.

8.2 Green alternatives of Organic Synthesis: Coenzyme catalysed reactions, thyamine catalyzed benzoin condensation. Green alternatives of Molecular rearrangements: Pinacol-pinacolone and Benzidine rearrangement. Electrophilic aromatic substitution reactions. Oxidation-reduction reactions. Clay catalysed synthesis. Condensation reactions. Green photochemical reactions.

8.3 Green Solvents: ionic liquids, supercritical CO_2, fluorous chemistry.

8.4 General principles of Microwave and Ultrasound assisted Organic Synthesis

References

01. M.B. Smith, Organic Synthesis, 3rd Edition, Wavefunctions Inc., 2011.

02. F.A. Carey, R.I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2009.

03. S. Warren, Organic Synthesis: The Disconnection Approach, John Wiley & Sons, 2004.

04. V.K. Ahluwalia, Oxidation in Organic Synthesis, Ane Books, 2012.

05. J. Tsuji, Palladium Reagents and Catalysts: New Perspectives for the 21st Century, John Wiley & Sons, 2003.

06. I. Ojima, Catalytic Asymmetric Synthesis, 2nd Edn., Wiley−VCH, 2000.

07. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.

08. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.

09. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

10. L. Kuerti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

11. R.O.C. Norman, J.M.Coxon, Principles of Organic Synthesis, ELBS and Chapmann and Hall, 1995.

12. V.K. Ahluwalia, L.S. Kumar, S. Kumar, Chemistry of Natural Products, Anne Books, 2009.

13. J.M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, 1995.

14. F. Vogtle, Supramolecular Chemistry: An Introduction, John Wiley & Sons, 1993.

15. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.

16. V. K.Ahluwalia, Green Chemistry: Environmently Benign Reactions, Anne Books, 2009.

AP3C10 CHEMISTRY AND BIOCHEMISTRY OF FATTY ACIDS

Credit : 4 **Contact Lecture Hours: 72**

Unit 1: Lipids (9 Hrs)

1.1 Classification of lipids-sources and classification of oils and fats, nomenclature of triglycerides, stereospecific numbering

1.2 Nutritional functions of fats and oils, Caloric and non caloric functions, Non nutritional functions of edible fats.

Unit 2: Isolation and Characterization of Fatty Acids (9 Hrs)

2.1 Crystallisation methods, Chromatographic techniques: TLC, paper chromatography, GLC, HPLC. Use of IR, UV, NMR and mass spectrometry.

2.2 Nomenclature of fatty acids- IUPAC and omega reference systems, uses of fatty acids in textiles, leather, pharmaceuticals and petroleum processing.

Unit 3: Fatty Acids Occurring in Nature (18 Hrs)

3.1 Saturated fatty acids: important sources, structure and synthesis of naturally occurring straight chain and branched chain saturated fatty acids.

3.2 Unsaturated fatty acids: monoethenoid fatty acids-their occurrence and general methods of synthesis. Oleic acid and petroselenic acid-properties and constitution, other monoethenoid acids occurring in animal and vegetable oils and fats.

3.3 Polyunsaturated fatty acids, cyclopropenoid acids, conjugated acids, epoxy acids, keto acids, cyclopentenoid acids, hydroxy acids, acetylenic acids, furanoid acids, artificially produced fatty acids, synthetic fatty acids.

Unit 4: Physical properties of Fatty Acids (9 Hrs)

4.1 Crystal properties, thermal properties, spectral properties, solubility and solution properties of fatty acids in the liquid state.

Unit 5: Chemical properties of Fatty Acids (18 Hrs)

5.1 Salt formation, esterification, halogenation, oxidation uses of various oxidizing agents like chromic acid, ozone, peroxides, potassium permanganate, periodic acid and lead tetra acetate. Hydrogenation, dehydration, pyrolysis, polymerization, addition reactions to double bond.

Unit 6: Biochemistry and Metabolism of Fats (9 Hrs)

6.1 Biochemical transformation of fats in the body-biosynthesis of fats in plants and animal organisms.

6.2 Prostaglandins: synthesis, biosynthesis, applications of prostaglandins as drugs.

References

01. M.G. Wohl, R.S. Goodhart, M.E. Shils, Modern Nutrition in Health and Disease, 6th Edn., Lea & Febiger, 1980.

02. K.S. Markley, Fatty acids: Their Chemistry, Properties, Production and Uses, Parts I- V, Interscience, 1960.

03. D. Swern, Bailey's Industrial oil and Fat Products, Vol. I-II, 4th Edn., John Wiley & Sons, 1982.

04. T.H. Aplewhite, Bailey's Industrial Oil and Fat Products, Vol.III, 4th Edn., John Wiley-Interscience,1985

05. T.P. Hilditch, P.N. Williams, The Chemical Constitution of Natural Fats, 4th Edn., John Wiley & Sons, 1964

06. F.D. Gunstone, An introduction to Chemistry and Biochemistry of Fatty acids and their Glycerides, Chapman and Hall, 1968.

07. H.B. Bull, The Biochemistry of Lipids, John Wiley, 1937.

08. T. Galliard, E.I. Mercer, Recent Advances in the Chemistry and Biochemistry of Plant Lipids, Academic Press, 1975.

09. F.D. Gunstone, Topics in Lipid Chemistry, Vol.I-II, Logos Press, 1970.

10. H.M. Sinclair, Essential Fatty Acids, Butterworths, 1958.

11. E.E. Conn, P.K. Stumpf, G. Bruening, R.H. Doi, Outlines of Biochemistry, 5th Edn., John Wiley, 1987.

AP3C11 ESSENTIAL OILS AND AROMATICS

Credit: 4 **Contact Lecture Hours:72**

Unit 1: Production and isolation of Essential Oils (9 Hrs)

1.1 Production of essential oils, Methods of isolation-Hydrodistillation, Solvent extraction, Enfleurage, Maceration, Expression, Supercritical fluid extraction.

Unit 2: Sources, Nature and Uses of Essential Oils (18 Hrs)

2.1 Study of the sources, production, general nature and use of the following essential oils: Lemongrass oil, Lemon oil, Citronella oils, Bergamot oil, Neroli oil, Palmarosa oil, Rosemary oil, Campher oil, Eucalyptus oil, Turpentine oil, Jasmine oil, Lavender oil, Rose oil, Geranium oil, Sandal wood oil, Clove oil, Cinnamon oil, Vetiver oil, Peppermint oil.

Unit 3: The Origin and Function of Essential Oils in Plants (9 Hrs)

3.1 Classification of Terpenoids, Isoprene rule, Physical and Chemical methods used for the investigation of essential oils and determination of the structure of terpenoids.

3.2 Biosynthesis of terpenoids, Formation of Mevalonic acid as intermediate, Biosynthesis of Monoterpenoids and Sesquiterpenoids.

Unit 4: Study of Essential Oil Constituents (36 Hrs)

4.1 Production, chemistry, classification, properties, reaction and synthesis of essential oil constituents with reference to the following:

Hydrocarbons: Ocimene, p-Cymene, Limonene, Carene, Pinene, Camphene, Fenchene, Bisabolene, Zingiberiene, Caryophyllene.

Alcohols: Linalool, Geraniol, Citronellol, Terpineol, Menthol, Borneol, IsoBorneol, Fernesol, Fenchyl Alcohol, Sandalols, Leaf alcohol.

Aldehydes: Citral, Citronellal, hydroxycitronellal.

Ketones: Methyl Heptenol, Menthone, Piperitone, Pulgone, Carvone, Fenchone, Campher, Ionones, Irones.

4.2 Spectral studies of the following compounds using UV-Visible, IR and Mass Spectrometry: Ocimene, Citral, Geraniol, Campher, Zingiberiene, Alpha Pinene, Pulgone, Piperitone, Ionone and Carvone.

References

1. E. Guenther, The Essential Oils, Vol I-VI, D.Van Nostrand, 1948.

2. A.A. Newman, The Chemistry of Terpenes and Terpenoids, Academic Press, 1972.
3. V. K. Ahluwalia, Terpenoids, Ane Books, 2009.
4. Y. Masada, Analysis of Essential Oils by Gas Chromatography and Mass Spectrometry, Wiley, 1976.
5. J.L. Simonson, The Terpenes, Vol.5, University Press, 1957.
6. A.R. Pinder, The Chemistry of Terpenes, Chapman and Hall, 1960.
7. J. Varghese, Terpene Chemistry, Tata McGraw Hill, 1982.
8. P. De Mayo, Mono and Sequiterpenoids, Interscience, 1969.
9. P.Z. Bedoukian, Perfumery Synthetics and Isolates, LCC, 2012.

AP3C12 SPECTROSCOPIC METHODS IN CHEMISTRY

Credit : 3 **Contact Lecture Hours: 54**

Unit 1: Ultraviolet-Visible and Chirooptical Spectroscopy (9 Hrs)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions. Chirooptical properties-ORD, CD, octant rule, axial haloketone rule, Cotton effect.

1.3 Problems based on the above topics.

Unit 2: Infrared Spectroscopy (9 Hrs)

2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.

2.3 Problems on spectral interpretation with examples.

Unit 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling-epi, peri and bay effects. NOE. NOE and cross polarization.

3.3 Simplification non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling.

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer. Selective Population Inversion. DEPT, INEPT and RINEPT. Sensitivity enhancement and spectral editing, MRI.

3.6 Problems on spectral interpretation with examples.

Unit 4: Mass Spectrometry (9 Hrs)

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, PD, Field Desorption Electrospray Ionization. Fragmentation

patterns-nitrogen and ring rules. McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Unit 5: Structural Elucidation Using Spectroscopic Techniques (9 Hrs)

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^{1}H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR and NMR spectra.

References

01. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole, 2000.

02. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, 1996.

03. L.D. Field, S. Sternhell, J.R. Kalman, Organic Structures from Spectra, 4th Edn., John Wiley & sons, 2007.

04. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

05. D.F. Taber, Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, Oxford University Press, 2007.

06. H. Gunther, NMR Spectroscopy, 2nd Edn., Wiley, 1995.

07. R.M. Silverstein, G.C. Bassler, T.C. Morril, Spectroscopic Identification of Organic Compounds, 5th Edn., Wiley, 1991.

08. D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6th Edn., McGraw-Hill, 2008.

09. W. Kemp, Organic Spectroscopy, 2nd Edn., Macmillan, 1987.

10. F. Bernath, Spectra of Atoms and Molecules, 2nd Edn., Oxford University Press, 2005.

11. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.

12. Online spectral databases including RIO-DB.

SEMESTER 4
ELECTIVE COURSES

(Any 3 courses to be opted from the following courses)

AP4E01 FATS, OILS AND WAXES

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Extraction of oils and fats (9 Hrs)

1.1 Mechanical pretreatment and heat treatment of oil bearing materials. Rendering of animal fats and cooking of oil seeds. Mechanical expression of oils. Solvent extraction-theory and practice, type of extractors, solvent recovery, alternative solvents for extraction, super critical fluid extraction of oils and fats. Newer methods in extraction of oils.

Unit 2: Commercially important oils and fats (18 Hrs)

2.1 Study of the sources, composition, characteristics and utilization of commercially important oils and fats-butter, tallow, lard, coconut oil, palm oil, palm kernel oil, peanut oil, cocoa butter, olive oil, cotton seed oil, rice bran oil, sesame oil, soybean oil, sunflower oil, tung oil, linseed oil, mustard oil, castor oil, hydnocarpus oil, marine oils.

Unit 3: Oils and fats as food materials (9 Hrs)

3.1 Cooking oil, salad oil, and salad dressings. Quality evaluation of cooking oils and salad oils. Margarine and Shortenings

3.2 Essential fatty acids: ω-3 and ω-6 fatty acids and their dietary sources, significance to human nutrition and health.

3.3 Fat-related diseases: atherosclerosis, arthritis. Nutritional significance of EFA, HDL, LDL and VLDL.

Unit 4: Glyceride structure (9 Hrs)

4.1 Glyceride composition of natural fats. Methods of investigation of glycerides. Theories of glyceride structure

Unit 5: Analysis of fats and oils (18 Hrs)

5.1 Test methods for physical properties: melting point, softening point, slipping point, titer, congeal point, flow test, cloud test, consistency test, penetration method, liquid and solid fatty acid determination, solid fat index, specific gravity, refractive index, viscosity, color, odor.

5.2 Test methods for chemical properties: Iodine value, thiocyanogen number, saponification value, acid value and free fatty acid, oxirane oxygen, hydroxyl and

acetyl value, peroxide value, Reichert-Meissel value, Polenski value and Kirschner value, diene value. Estimation of poly unsaturated fatty acids-Kries test, thiobarbituric acid test

5.3 Adulteration of oils fats – detection of adulteration

Unit 6: Nonglyceride constituents of fats and oils (9 Hrs)

6.1 Occurrence, chemistry and function of carotenes, vitamins, tocopheols, steroids, phospholipids, sphingolipids, antioxidants. Constituents contributing flavor and odor.

Unit 7: Waxes and Fatty Alcohols (9 Hrs)

7.1 Occurrence, classification, properties and composition of waxes. Synthetic waxes. Analysis and utilization of waxes.

7.2 Naturally occurring fatty alcohols-production, uses and applications. Alcohol ethers.

Unit 8: Rancidity in oils, fats and oil bearing substances (9 Hrs)

8.1 Concept of autoxidation, theories of autoxidation, tests for rancidity, stability of oils, induction period, Pro oxidants and antioxidants, drying, semidrying and nondrying oils.

References

01. D. Swern, Bailey's Industrial oil and Fat Products, Vol. I-II, 4th Edn., John Wiley & Sons, 1982.

02. T.H. Aplewhite, Bailey's Industrial Oil and Fat Products, Vol.III, 4th Edn., John Wiley-Interscience,1985

03. F.D. Gunstone, An introduction to Chemistry and Biochemistry of Fatty acids and their Glycerides, Chapman and Hall, 1968.

04. T.P. Hilditch, P.N. Williams, The Chemical Constitution of Natural Fats, 4th Edn., John Wiley & Sons, 1964

05. H.A. Boekenoogen, Analysis and Characterization of Oils, Fats and Fat Products, Vol.I, Interscience, 1964.

06. P. Tooley, Chemistry in Industry-Fats, Oils and Waxes, John Murray, 1971.

07. W.W. Christie, Lipid Analysis, 3rd Edn., Oily Press, 2003.

AP4E02 INDUSTRIAL OIL AND FAT PRODUCTS

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Processing of Oils and Fats (9 Hrs)

1.1 Refining, bleaching, deodorization, fractionation, winterization, stabilization, solidification, homogenization, emulsification and dewaxing.

Unit 2: Hydrogenation of Oils (9 Hrs)

2.1 Catalytic hydrogenation: chemistry of hydrogenation, hydrogenolysis, influence of various factors in hydrogenation, mechanism, kinetics and thermodynamics of hydrogenation reactions, hydrogenation catalysts-theory of catalysis, materials and apparatus, new developments in plants and processes for hydrogenation.

2.2 Industrial processes of: -

a) Manufacture of catalyst for hydrogenation, hydrogen production and purification.

b) Hydrogenation of vegetable and marine oils-manufacture of vanaspati.

c) Reduction of long chain fatty acids.

Unit 3: Fat Splitting and Esterification (18 Hrs)

3.1 Fat splitting: Twitchell process, low pressure splitting with catalysts, medium pressure autoclave splitting with catalyst, continuous uncatalyzed high pressure counter current splitting, enzymatic splitting, recovery of glycerine from fat splitting process and spent lye, different grades of glycerine, chemistry and synthesis of glycerine, uses of glycerine, glycerine substitutes.

3.2 Esterification: mechanism of esterification and ester hydrolysis, esterification of fatty acids with glycerol and other alcohols, inter esterification, acidolysis, alcoholysis, glycolysis, glycerolysis, transesterification and its mechanism, applications of esterification and inter esterification.

Unit 4: Theories of Surface Action (9 Hrs)

4.1 Applications of surface active agents, liquid-gas interfaces, liquid-liquid interfaces, liquid-solid interfaces, boundaries between three phases, foaming and defoaming, emulsification, wetting of solids, adsorption on solid surfaces, detergency.

Unit 5: Soaps (9 Hrs)

5.1 Soap manufacture: raw materials, characteristics of cold process, semi boiled process and boiled process, additives of soap, detergent action of soap, influence of fatty acid composition of the oil on properties of soap, manufacture of soap for different purposes-laundry soaps, toilet soaps, liquid soaps, transparent soaps,

baby soaps, shaving soaps, medicated soaps, textile soaps, naphtha soaps, marine soaps.

5.2 Chemical analysis of soaps- T.F.M value of soaps.

5.3 Shampoos.

Unit 6: Synthetic Detergents (9 Hrs)

6.1 Detailed study of the anionic, cationic, amphoteric and nonionic detergents used in modern industries and for household purposes-their chemistry, manufacture and applications. Agglomeration.

6.2 Merits and demerits of syndets over soaps, biodegradability of detergents

6.3 Role of surfactants in synthesis of nano particles, enzyme detergents, Green detergents, compact detergents.

Unit 7: Paints, Varnishes and Lacquers (9 Hrs)

7.1 Paints as protective coatings, paints and enamels, materials for paint manufacture, oils used-unmodified oils and their pretreatment, modified drying oils, resins and copolymers-natural resins, phenolic resins, alkyd resins, urethane resins, epoxy resins.

7.2 Driers, thinners, pigments and miscellaneous ingredients, mechanism of polymerization and drying of oils

7.3 Testing and evaluation of paints: density, viscosity, brushability, spraying properties, covering power, opacity, drying time, volatile content, flash point, optical and mechanical properties of dry films.

7.4 Varnishes and lacquers: composition and uses, oleoresinous varnishes, defects in varnish films.

7.5 Control of volatile organic emissions in paint industry.

Unit 8: Miscellaneous Oil and Fat Products (9 Hrs)

8.1 Sulphonated oils-sulphonation process, applications of sulphonated oils.

8.2 Linoleum, oiled fabrics, lubricants and plasticizers, illuminants and fuels.

Unit 9: Instrumental Analysis of Oil and Fat Products (9 Hrs)

9.1 Applications of a) Refractometry b) Dilatometry c) Polarography d) X-ray diffraction.

References

01. D. Swern, Bailey's Industrial Oil and Fat Products, Vol. I and II, 4th Edn., John Wiley, 1982.

02. T.H. Applewhite, Bailey's Industrial Oil and Fat Products, Vol.III, 4th Edn., John Wiley, 1985.

03. E.S. Pattison, Fatty acids and their Industrial Applications, Marcel Dekker, 1968.

04. A.J.C. Andersen, Refining for Oils and Fats for Edible Purposes, Pergamon Press, 1962.

05. C.R. Martens, Emulsion and Water soluble Paints and Coatings, Reinhold, 1964.

06. L.I. Osipow, Surface Chemistry-Theory and Industrial Applications, R E Krieger, 1972.

07. M. Ash, I. Ash, Formulary of Detergents and Other Cleaning Agents, Chemical Publishing, 1999.

08. W.M. Morgans, Outlines of Paint Technology, Wiley, 1990.

AP4E03 CHEMISTRY OF AROMATICS AND ESSENTIAL OIL CONSTITUENTS

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Spices (**18 Hrs)**

1.1 Study of the sources, production, nature, chemical constituents and uses of common spices and condiments such as Cardamom, Pepper, Clove, Nutmeg, Mace, Cinnamon, Ginger, Turmeric, Celery, Fennel, Fenugreek, Coriander, Garlic, Vanilla, Saffron, Allspices, Curry leafs, Mint and Mustard.

Unit 2: Spice Oils and Oleoresins (**9 Hrs)**

2.1 Methods of production, chemistry of the constituents and uses of the following: Pepper, Ginger, Turmeric.

Unit 3: Production and Chemistry of Aromatics and Essential Oil Constituents (36 hrs)

3.1 Natural Source, production and chemistry of aromatics and essential oil constituents such as:

a) Alcohols: Benzyl alcohol, Phenylethyl alcohol, Cinnamyl alcohol.

b) Aldehyde: Benzaldehyde, Phenylacetaldehyde, Cinnamic aldehyde, Salicylaldehydes, Anisaldehyde, Vanillin, Piperonal.

c) Phenols: Thymol, Carvacrol, Eugenol, Isoeugenol, Methyleugenol.

d) Acids and Esters: Benzoic acid, Cinammic acid, Salicylic acid, Anisic acid, Anthranilic acid, Phenylacetic acid, Benzylacetate, Benzylbenzoate, Cinnamylacetate, Geranylacetate, Linalylacetate, Menthylacetate, Amylacetate.

e) Miscellaneous Compounds- Coumarin, Cineoles, Anethole, Ascaridole, Indole, Muscone, Civetone, Exalton, Artificial Musk.

Unit 4: Flavour (**9 Hrs)**

4.1 Concept of flavor, difference between perfumes and flavour. Flavour Characterisation.

4.2 Sensory analysis-descriptive and discriminent Sensory Analysis.

4.3 Flavour of Coffee, Tea, Cocoa, Onion and Garlic. Synthetic ingredients of food flavourings.

Unit 5: Perfumes **(18 Hrs)**

5.1 Odour, Odorants, Olfaction, Classification of odour. General Physiology of Olfaction.

5.2 Perfume Raw materials-Terpeneles and Sesqueterenles oils, Concrete oils, Absolute oils, Isolates from essential oils, Tincture, Balsams and Resins.

5.3 Source and Chemical nature of commercially important Gums, Balsams and Resins.

5.4 Perfume Technology-blending and formulation of perfumes. Aerosol Spray Perfumes.

References

01. F. Rosengarten, The Book of Spices, Jove, 1981.

02. J.W. Parry, Hand Book of Spices, Chemical Publishing, 1969

03. J.S. Pruthi, Spices and Condiments Chemistry, Microbiology and Technology, Academic Press, 1980.

04. E. Guenther, The Essential Oils, Vol I-VI, Van Nostrand, 1972.

05. M. Billot, F.V. Wells, Perfumery Technology: Art, Science and Industry, E. Horwood, 1975.

06. E.T. Theimer, Fragrance Chemistry: the Science of the Sense of Smell, Academic Press, 1982.

07. L. Appell, Cosmetics, Fragrances and Flavours, Novox, 1982.

08. N. Groom, The Perfume Handbook, Chapman and Hall, 1992.

09. L.H. Meyer, Food Chemistry, Reinhold, 1960.

AP4E04 ANALYTICAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Unit 1: Instrumental Methods (36 Hrs)

1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods-precision, sensitivity, selectivity, and detection limits.

1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio-hardware and software methods.

1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

1.4 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments-sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.

1.5 Molecular fluorescence and fluorometers: photoluminiscence and concentration-electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Introduction to photoacoustic spectroscopy.

1.6 IR spectrometry: instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR instruments. Mid IR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.

1.7 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.

1.8 NMR Spectrometry-magnets, shim coils, sample spinning, sample probes (^{1}H, ^{13}C, ^{32}P). Principle of MRI.

Unit 2: Sampling (18 hrs)

2.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non essential water, absorbed and occluded water, determination of water (direct and indirect methods).

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions. Types of extraction procedures.

Unit 3: Applied Analysis **(9 hrs)**

3.1 Analytical procedures involved in environmental monitoring. Water quality-BOD, COD, DO, nitrite, nitrate, iron, fluoride.

3.2 Soil-moisture, salinity, colloids, cation and anion exchange capacity.

3.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 and SPM.

3.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis.

Unit 4: **Capillary Electrophoresis and Capillary Electro-chromatography** **(9 Hrs)**

4.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection(indirect)-fluorescence, absorbance, electrochemical, mass spectrometric, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.

4.2 Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography.

Unit 5: Process instrumentation **(9 Hrs)**

5.1 Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N analysers.

Unit 6: Aquatic Resources **(9 Hrs)**

6.1 Aquatic resources: renewable and non renewable resources, estimation, primary productivity and factors affecting it, regional variations.

6.2 Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion exchange and hydrate formation methods. Relative advantages and limitations. Scale formation and its prevention in distillation process.

6.3 Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of chemicals, salt from solar evaporation.

References

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

02. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.

03. R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.

04. H.H. Willard, L.L. Merritt, J.A. Dean, Instrumental Methods of Analysis, Van Nostrand, 1974.

05. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.

06. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
07. J.G. Dick, Analytical Chemistry, R.E. Krieger, 1978.
08. E.D. Howe, Fundamentals of Water Desalination, Marcel Dekker, 1974.
09. H.G. Heitmann, Saline Water Processing, VCH, 1990.

SEMESTERS 3 AND 4

AP4P04 INDUSTRIAL OIL AND FAT PRODUCTS PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

I. Preparation of samples of refined and bleached oils.

II. Analysis of vanaspati:
   1. Determination of the physical and chemical constants of hydrogenated fats.
   2. Estimation of residual nickel catalyst in hydrogenated fats.
   3. Estimation of Vitamin A and Vitamin E content of vanaspati.
   4. Determination of isooleic acids in hydrogenated fats.
   5. Detection of animal fats in vanaspati.
   6. Estimation of nickel in catalyst mixture and spent catalyst.

III. Soap analysis:
   1. Complete analysis of washing soaps, toilet soaps and transparent soaps: moisture, alcohol soluble and insoluble's, free caustic alkali, combined alkali, anhydrous soap, titer, mean molecular weight and Iodine value of total fatty acids derived from soaps.
   2. TFM value of toilet soaps.
   3. Estimation of glycerine content of toilet soaps and transparent soaps.
   4. Test for detection of rosin in soaps. Estimation of rosin in soaps.
   5. Analysis of soap stock-acidulated and neutral oil.
   6. Analysis of spent lye: Estimation of glycerine, total alkali and sodium chloride in spent lye.

IV. Glycerine analysis: Analysis of glycerine for specifications-glycerine content, ash, total residue, acidity/alkalinity.

V. Analysis of detergent powders:

   a) Preparation of different types of soap-washing soap, toilet soap, transparent soap, liquid soap, shaving soap.

   b) Preparation detergent powder, shampoo, vanishing cream.

References

01 F. Shahidi, Bailey's Industial Oil and Fat Products, 6th Edn., John Wiley & Sons, 2005.

02. I. Ash, M. Ash, Formulary of Detergents and other Cleaning Agents, Chemical Publishing, 1999

03. H. Butler, Poucher's Perfumes, Cosmestics and Soaps, 10th Edn., Springer, 2000.

AP4P05 ESSENTIAL OILS AND AROMATICS PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

I. Experiments to illustrate the preparation of essential oils by (a) steam distillation (b) solvent extraction (c) effleurage.

II. Assay of essential oils and perfumery materials: Determination of specific gravity, refractive index, optical rotation, boiling point and boiling range. Fractionation and solubility. Estimation of essential oil constituents such as alcohols, esters, aldehydes, ketones, phenols and others.

Examples-

01. Estimation of acids in essential oils.
02. Geraniol in palmarosa oil.
03. Citronellol in citronella oil.
04. Linalool in bergamot or lavender oil.
05. Citral in lemongrass oil.
06. Citronellal in citronella oil.
07. Cinnamic aldehyde in cinnamon oil.
08. Methyl salicylate in wintergreen oil.
09. Geranyl acetate in palmarosa oil.
10. Camphor in camphor oil.
11. Cineole in eucalyptus oil.
12. Eugenol in clove oil.
13. Estimation of vanillin.
14. Estimation of aldehydes and ketone components in a mixtrure.

III. Estimation of essential oil content in oil bearing materials.

IV. Detection and estimation of common adulterants such as alcohol, rosin, fatty oil and mineral oil in essential oils.

V. Determination of ethyl alcohol content in tinctures and essences.

VI. Preparation of some typical isolates from essential oils.

01. Citral from lemongrass oil.
02. Geraniol from palmarosa oil.
03. Santalols from sandalwood oil.
04. Cineol from eucalyptus oil.
05. Linalool from bergamot oil.

06. Cinnamic aldehyde from cinnamon oil.

07. Eugenol from clove oil.

VII. Synthesis of aromatics and perfumery compounds:

01. Nerolin.
02. B- ionone.
03. Methyheeptenone.
04. Camphor.
05. Methl cinnamate.
06. Methyl anthranilate.
07. Benzyl acetate.
08. Amyl benzoate.
09. Coumarin.
10. Amy isovalerate.
11. Amyl salicylate.

References

01. E. Guenther, The Essential Oils-Vol.1, Jepson Press, 2007.

02. W.A. Poucher, Perfumes, Cosmetics and Soaps, 9th Edn., Springer, 1993.

03. M. Billot, F.V. Wells, Perfumery Technology: Art, Science, Industry, E. Horwood, 1975.

04. J.S. Pruthi, Spices and Condiments: Chemistry, Microbiology, Technology, Academic Press, 1980.

05. R.F. Venn, Principles and Practice of Bioanalysis, Taylor& Francis, 2007.

06. G. Reineccius, Flavour Chemistry and Technology, 2nd Edn., 2005.

AP4P06 FIXED OILS AND FATS PRACTICAL

Credit: 3 **Contact Lab Hours: 72+72=144**

I. Determination of the physical and chemical constants of common oils and fats.

II. Moisture, Specific gravity, Refractive index, Acid value and free fatty acid, Saponification value, Iodine value, Non-saponifiable matter, Acetyl and hydroxyl value, Reichert Meissl value, Polenske and Kirschner value, peroxide value and color measurement of the following:

01.Coconut oil.
02.Sesame oil.
03.Palm oil.
04.Olive oil.
05.Castor oil.
06.Peanut oil.
07.Soya bean oil.
08.Rice bran oil.
09.Mustard oil.
10.Hydnocarpus oil.
11.Shark liver oil.
12.Ghee.
13.Tallow.

III. Kauffmann's Thiocyanogen value-Determination of linoleic and linolenic acids in fats.

IV. Special test for oils: Stoke's test and Bailey's test for Castor oil, test for detection of Peanut oil, color test for cotton seed oil and sesame oil.

V. Detection of common adulterants in oils and fats. Detection of vanaspati in butter and ghee.

VI. Assessment of the quality of fats-Preparation of the total fatty acids and determination if its iodine value, titer and mean molecular weight.

VII. Separation and estimation of saturated acid in mixtures and in oils-Bertram method and lead salt method.

VIII. Investigation of the fatty acid composition of the oils and fats, Preparation of total fatty acids, Esterification-Ester fractionation by chromatographic method-Separation and analysis of fatty acids.

IX. Analysis of oil cake: Estimation of (a) residual oil and (b) protein nitrogen.

X. Estimation of total phospholipids in oils containing nonglyceride constituents. Estimation of phosphorous in lecithin.

XI. Colorimetric estimation of cholesterol in fats.

XII. Preparation based on oils and fats: Preparations involving epoxidation, hydroxylation, bromination and chain scission of fatty acids. Isolation of individual fatty acids from oils.

Examples:

1. Epoxystearic acids.
2. Erythro-9, 10-dihydroxystearic acid.
3. threo-9, 10-dihydroxystearic acid.
4. Tetrabromostearic acid.
5. Azelaic acid.
6. Sebacic acid.
7. Undecylenic acid.
8. Isolation of palmitic acid from palm oil.
9. Isolation of erucic acid from mustard oil.

XIII. Preparation of rice bran oil by solvent extraction method.

References

01 V.C. Mehlenbacher, Official and Tentative Methods of the American Oil Chemists Society Vol.1, 3rd Edn., The Society, 1954.

02. H.A. Boekenoogen, Analysis and Characterization of Oils, Fats and Fat Products, Interscience, 1954.

03. L.V. Cocks, C.V. Rede, Laboratory Hand Book for Oil and Fat Analysis, Academic Press, 1966.

04. F.D. Gunstone, An Introduction to the Chemistry and Biochemistry of Fatty Acids and their Glycerides, Chapman and Hall, 1968.

05. F.D. Gunstone, Topics in Lipid Chemistry, Logos, 1970.