

M.Sc. SEMESTER - I
CHE402 Organic Chemistry

Unit-1

(A) Elimination Reaction

The E₁, E₂, E₁CB mechanism, stereochemistry. Orientation of the double bond *syn* and *anti* eliminations. Reactivity- effects of substrate structures, attacking base, leaving group and medium. Mechanism and orientation in pyrolytic *syn* eliminations – Chugaev and Cope eliminations.

(B) Nucleophilic Substitution Reaction

Mixed SN₁, SN₂ and SET mechanism.
Nucleophilic substitution at (a) Allylic carbon (Allylic rearrangements), (b) An Aliphatic trigonal carbon (the tetrahedral mechanism) and at (c) A Vinyl carbon. Participation of Neighboring groups in Nucleophilic substitution by (a) Carboxylate anion (b) Halogen atoms (c) Hydroxyl groups (d) Acetoxy group (e) Phenyl group (f) RS group (g) Participation by π -bond.

Unit-2

(A) Aromaticity

Aromaticity, aromatic character, Frost circle diagram for cyclobutadiene, benzene and others. Resonance and chemical stabilization-aromatic character based on NMR criteria, Huckels rule, energy level of π molecular orbitals, Huckels molecular orbital(HMO) method, MO of simple organic systems such as ethene, allyl and butadiene Aromaticity in benzenoid and non-benzenoid compounds and charged rings, annulenes, fulvenes, azulenes, antiaromaticity and homoaromaticity.

(B) Acid base concept, pK_a, Hammett equation, Concept of hindered base, The effect of structure on the strength of acids and bases.

Unit - 3

(A) Reactive intermediates

- (1) Carbocations (classical and non classical) stability, structure, generation and fate
- (2) Carbanions- stability, structure, generation and fate of carbanions
- (3) Carbenes- stability and structure, the generation and fate of carbenes.
- (4) Free radicals: stability, structure, generation and fate of free radicals, NBS
- (5) Nitrene : stability, structure, generation, reaction

(B) Rearrangements:

General mechanistic considerations, nature of migration, migratory aptitude, and memory effects in respect of following.

(1) Carbon to Carbon migration of R, H and Ar

- (i) Pinacol- Pinacolone rearrangement
- (ii) Favorskii rearrangement

(2) Carbon to Nitrogen migrations:

- (i) Curtius rearrangement
- (ii) Schmidt rearrangement

(3) Carbon to oxygen migration of and Ar

- (i) Baeyer- villiger rearrangement
- (ii) Rearrangement of hydroperoxide

Unit - 4

Stereo Chemistry

Optical and geometrical isomerism, origin of chirality and chiral centre, axis and plane, helicity, Enantiotopic and diastereotopic atoms, groups and faces, prochiral centre, biphenyl, allenes, spirans, compounds containing chiral nitrogen and sulfur, stereospecific and stereoselective synthesis, dynamic resolution.

M.Sc. SEMESTER – I
CHE402 Organic Chemistry : Theory

References:

- 1) Advanced Organic Chemistry, Reactions Mechanisms and Structure , J. March, 6th Edition, John Wiley.
- 2) Carbenes, nitrenes and arynes, T.L. Gilchrist and C.W. Rees.
- 3) Guidebook to Mechanism in Organic Chemistry by Peter Sykes, 6th Edition, Prentice Hall.
- 4) Advanced Organic Chemistry Part A: Structure and Mechanism and Part B: Reaction and synthesis ,Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer .
- 5) Organic Chemistry, Johnathan Clayden, Nick Greeves, Stuart Warren, 1st Edition, Oxford University Press.
- 6) Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, 3rd Edition, Blackie Academic and Professional.
- 7) Stereo Chemistry , P.S. Kalsi , New Age Publications.
- 8) Reagents in Organic Synthesis- Fieser and Fieser, John Wiley.
- 9) Physical Organic Chemistry by Jack Hynes,(plenum publication)
- 10) Organic Chemistry, T.W. Graham Solomons and Graig B. Frymes, John Wiley and Sons.
- 11) Organic Chemistry, F. A. Carey, McGraw Hill Edition.
- 12) General Organic Chemistry Sachin Kumar Ghose, New Central book agency.
- 13) Organic Chemistry Vol 1-2 I.L.Finar 5th edition,ELBS.

M.Sc. - Semester – I (PRACTICALS)
CHE405PR Organic Chemistry

Preparation of organic compounds :

- i) Nitration
- ii) Bromination
- iii) Acylation
- iv) Reduction
- v) Oxidation
- vi) Condensation reaction
- vii) Diazotization reaction
- viii) Friedl-Craft's reaction
- ix) Cannizzaro reaction
- x) Aldol condensation

Quantitative Estimations

- a. Estimation of ester + acid
- b. Estimation of formaldehyde
- c. Estimation of glycine
- d. Estimation of amide + acid

M. Sc. - Semester – I (PRACTICALS)
CHE405PR Organic Chemistry

References:

1. A text book of practical organic chemistry – A. I. Vogel
2. Practical organic Chemistry – Mann and Saunders
3. A handbook of quantitative and qualitative analysis – H. T. Clarke
4. Comprehensive Practical Organic Chemistry : Qualitative Analysis V K Ahluwalia & S. Dhingra.
5. Comprehensive Practical Organic Chemistry : Preparations and Quantitative Analysis V K Ahluwalia & R. Aggarwal Universities Press.
6. An Advance Course in practical Chemistry, A K. Nad, B. Mahapatra and A. Ghoshal.

M.Sc. SEMESTER II
CHE408 Organic Chemistry

Unit-1

Spectroscopy

- 1) ¹³C NMR : General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants.
- 2) Mass spectroscopy : Introduction, ion production, EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectroscopy.
- 3) Examples of mass spectral fragmentation of organic compounds, NMR, IR, UV with respect to their structure determination.

Unit - 2

(A) Photochemistry:

- (1) Photochemical reactions: Principles of energy transfer, electronic excitation and molecular orbital view of excitation, excited states and fate of excited molecules (modified Jablonski diagram), Photosensitization.
- (2) Photochemistry of carbonyl compounds: Representation of excited states of ketones, photoreduction Norrish type I & II reactions, Reactions of cyclic Ketone, oxetane formation (Paterno-Buchi reaction)
- (3) Di- π methane rearrangement, Dienone photochemistry, cis-trans isomerisation and photochemistry of conjugated olefins.

(B) Chemistry of Heterocycles

- (1) Nomenclature of heterocycles : Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles. General chemical behavior of aromatic heterocycles.
- (2) Five-membered and benzo fused five member heterocycles : Oxazole, Isoxazole, Thiazole, Pyrazole, Imidazole, Benzothiazole and Benzimidazole.
- (3) Six membered and benzofused six membered heterocycles : Pyrazine, Pyridazine, Pyrimidine, Cinnoline, Quinazoline, Quinoxaline, Phenoxaline.

Unit - 3

Name reactions : General nature, method, mechanism and synthetic applications of the following reactions:

- (i) Vilsmeier-Haack reaction
- (ii) Mitsunobu reaction
- (iii) Suzuki reaction
- (iv) Buchwald Hartwig reaction (cross coupling)
- (v) Sonogashira coupling
- (vi) Stobbe condensation
- (vii) Jones oxidation
- (viii) Swern oxidation reaction
- (ix) Michael addition
- (x) Darzen's glycidic ester synthesis
- (xi) Mannich reaction
- (xii) Dickmann reaction
- (xiii) Birch reduction
- (xiv) Wittig reaction
- (xv) Knoevenagel reaction

Unit-4

Reagents in organic synthesis : Mechanism selectivity and utility of following reagents:

- (i) Gilman's reagent-Lithium dimethylcuprate
- (ii) Lithium diisopropylamide (LDA)
- (iii) Dicyclohexyl carbodiimide (DCC)
- (iv) 1,3 – Dithiane (Umpolung reagent)
- (v) Dess- Martin periodinane
- (vi) Bakers yeast
- (vii) Diisobutylaluminium hydride(DIBAL –H)
- (viii) Sodium cyanoborohydride (NaBH₃(CN))
- (ix) Grignard reagents
- (x) Sodium borohydride
- (xi) DDQ
- (xii) n-Butyl lithium
- (xiii) Phase transfer catalysis : Quaternary ammonium and phosphonium salts, crown ethers.

M.Sc. SEMESTER II - Theory

CHE408 Organic Chemistry

References

- 1) Modern Synthetic Reactions, H.O.House, W.A. Benjamin.
- 2) Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, 3rd Edition, Blackie Academic and Professional.
- 3) Spectrometric Identification of Organic Compounds by Robert M. Silverstein, 7th Edition, Wiley.
- 4) Mass Spectrometry – A Textbook Jurgen Gross, 1st Edition, 2002, Springer – Verlag Berlin Heidelberg.
- 5) Introductory Photochemistry, A.Cox and T.Camp, McGraw Hill.
- 6) Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
- 7) Organic Photochemistry, J. Coxon and B. Halton, 2nd Edition, Cambridge University Press.
- 8) Strategic Applications of Named Reactions in Organic Synthesis, Laszlo Kurti and Barbara Czak, 1st Edition, Academic Press.
- 9) Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, Michael G. Ellerl, Frank G. Favalaro, 2nd Edition, Wiley – Interscience.
- 10) Name Reactions. A Collection of Detailed Reaction Mechanisms., Jie Jack Li, 3rd Edition, Springer.
- 11) Heterocyclic Chemistry, volume 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer- Verlag.
- 12) Heterocyclic Chemistry, J.A. Joule, K.Mills, and G.F. Smith, 3rd Edition, Chapman and Hall.
- 13) Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
- 14) Contemporary Heterocyclic Chemistry, G.R. Nikome and W.W. Poudler, Wiley.
- 15) Comprehensive Heterocyclic Chemistry, A.R. Kartizky, and C.W. Rees.
- 16) Encyclopedia of Reagents for Organic Synthesis, Leo A. Paquette, David Crich and Phillip L. Fuchs, John Wiley and Sons Inc.
- 17) Organic Chemistry, T.W. Graham Solomons and Graig B. Frymes, John Wiley and Sons.
- 18) Organic Chemistry, F. A. Carey, McGraw Hill Edition.
- 19) General Organic Chemistry Sachin Kumar Ghose, New Central book agency.
- 20) Guidebook to Mechanism in Organic Chemistry by Peter Sykes, 6th Edition, Prentice Hall.
- 21) Advanced Organic Chemistry Part A: Structure and Mechanism and Part B: Reaction and synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer.
- 22) Organic Chemistry Vol 1-2 I.L.Finar 5th edition, ELBS.

M.Sc Semester – II (PRACTICALS)

CHE411PR Organic Chemistry

Mixture analysis: ternary mixture to be given. (S+S+S) or (L+L+L). Type determination. Separation by physical and chemical methods. (both permitted in case of liquids)

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