

JNTUH COLLEGE OF ENGINEERING HYDERABAD

PhD course work

L	T	P	C
4	0	0	4

CHEMISTRY OF SYNTHETIC REAGENTS & PATENT RIGHTS (OCY 15 302)

Objectives: The knowledge of oxidizing and reducing reagents is required for the student. The student should know the requirements and procedures for filing the patents, which is very important.

Unit - 1: Oxidizing & Dehydrogenating Agents:

Oxidizing agents used in Organic Synthesis – Chromium (VI) Oxidizing agents like Potassium dichromate, Chromium trioxide, Pyridinium Chlorochromate, Pyridinium dichromate. KMnO_4 , Manganese dioxide; hydrogen peroxide, m-chloroperbenzoic acid, peroxyacetic acid, DDQ, Lead Tetraacetate, Cupric acetate, Ceric ammoniumnitrate.

Unit - 2: Reducing Agents:

Sodium in alcohol; H_2 over Catalysts (heterogeneous and homogeneous); Raney Ni Magnesium in alcohol. Sodium borohydride, Lithium aluminiumhydride, Sodium Cyanoborohydride, Zn-Hg in HCl.

Unit - 3: New Synthetic Reagents:

Silicon compounds in organic synthesis, Allyl triethyl silanes, Diphenyl Silane, Benzyl trimethylsilane, Sulphur compounds for organic synthesis, Oxidizing agents, Swern oxidation, C-C bond formation using dithianes (1,3-dithiane), Phase Transfer Catalysts in organic synthesis, Quaternary Ammonium Compounds, Crown ethers, Phosphonium Compounds, Pyridinium compounds.

Unit - 4: Use of Organometallic Reagents:

C-C bond formation using Grignard reagents; alkyl and aryl lithium, Organo-copper reagents; Palladium in organic synthesis; Stille, Negishi Suzuki & Heck Coupling reactions. Grubbs' Metathesis reactions. Miyaura reactions, Mitsunobu reaction. C-N Bond formation-Buchwald-Hartwig reaction.

Unit - 5: Intellectual Property Rights & Patents:

Introduction to Patents, copy right, Trademarks. GIs, Patents in the wider context of intellectual property rights; What can be Patented, requirements for patentability, patent restrictions, how are patents obtained; Patent filing: The Power of Patents. Introduction to Patent Medicine; Role of patents in R & D.

Outcomes: A thorough knowledge of oxidizing and reducing agents, Silicon, Sulphur and Phase Transfer catalyst compounds in chemical synthesis obtained. The detailed principles, procedures and requirements for filing patents is gained from this course.

Books Recommended:

1. "Reagents for Organic Synthesis", Fieser and Fieser.
2. "Synthetic Reagents" Vols. I and II, Pizey.
3. "Organic Synthesis – Special Techniques", V.K. Ahluwalia & Renu Aggarwal, Narosa Publishing House, New Delhi (2001).
4. "Reactions, Rearrangements and Reagents", S.N. Sanyal, Bharati Bhawan, Publishers, Patna (2002).
5. "Organic Reaction Mechanisms", V.K. Ahluwalia & R. K. Parashar, Narosa Publishing House, New Delhi (2002).

6. "*What everyone should know about Patents*", N. Subbaram, Pharma Book Syndicate, Hyderabad (2003).
7. "*Name reactions*", K. Jack Lee
8. "*Organic Synthesis*", Curruthers Ritchard.
9. "*Organic Synthesis*", Carrey & Sund Berg Vol. I, Vol.II.
10. "*Organic Synthesis*", Michael B.Smith

JNTUH COLLEGE OF ENGINEERING HYDERABAD

L	T	P	C
4	0	0	4

ORGANIC SPECTROSCOPY (OCY 15 303)

Objectives: The spectroscopy is very important concept for the determination of structures of organic molecules. The basic principles of various types of spectroscopy viz., IR, NMR, Mass and their applications are to be learnt by the student.

Unit 1: Infra Red Spectroscopy:

Degrees of freedom for the energy of a molecule; Molecular Vibration – Types of molecular vibration; Mechanics of measurement of IR Spectra; Block Diagram of the IR Spectrometer; Sampling techniques; Factors influencing IR absorption peaks; Fermi Resonance, Coupling Interaction, Hydrogen bonding etc; Interpretation and applications of IR Spectra.

Unit 2: Nuclear Magnetic Resonance Spectroscopy – I:

Principles of NMR Spectroscopy; Characteristics of a PMR Spectrum; Number of signals; Chemical shift - Ring current effects Aromaticity, Diamagnetic Anisotropic effects; Integration, Spin-Spin coupling. Mechanics of Measurement; Instrumentation for Continuous wave PMR; Solvents used; Reference standards such as TMS, DSS etc.

Unit 3: Nuclear Magnetic Resonance Spectroscopy – II:

Coupling constants; Karplus Equation; Vicinal, geminal, vinylic and aromatic protons. Nuclear Magnetic Resonance – A closer look; Larmor's Precessional Motion; Spin - Spin and spin-lattice Relaxations; Population of Nuclear spins; Protons bound to heteroatoms; Protons bound to Oxygen – Effect of hydrogen bonding & chemical exchange; Spectrum of ethanol; Protons bound to Nitrogen; Effect of nuclear quadrupole moment; D₂O exchange process; Hindered rotation; Spectrum of Dimethyl formamide.

Unit 4: Advanced Nuclear Magnetic Resonance Spectroscopy:

Simplification of PMR spectrum; Higher Resolution NMR; Double Resonance technique; Lanthanide shift reagents. ¹³C NMR Spectroscopy; CW & FT methods; Proton Noise Decoupled and Off-Resonance Spectra; 2D – NMR spectroscopy; NOESY & COESY Techniques.

Unit 5: Mass Spectrometry:

Basic principles; Instrumentation– The electron –impact mass spectrometer; GC-MS and Double Focussing instruments; Nitrogen rule, Types of ions in the mass spectrometer – Mass spectral fragmentation patterns of some select class of organic compounds such as hydrocarbons, alcohols, acids etc. - Mc Lafferty rearrangement, Methods of ionizations EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques- Applications.

Outcomes: The student will learn the principle involved in IR, NMR and Mass spectroscopic techniques in finding out the structures of organic compounds. The latest techniques like NOESY, COESY and advanced instrumentation like MALDI, GC-MS, LC-MS are learnt.

1. "*Spectrometric Identification of Organic Compounds*", R.M. Silverstein, G.C. Bassler and T.C. Morill, John Wiley & Sons, New York (1981).
2. "*¹³C – NMR Spectroscopy*", Abraham and Lofthus, Heydon & Sons Ltd., Philadelphia (USA) (1979).
3. "*Spectrometric Methods in Organic Chemistry*", Dudley H. Williams and Ian Flemming, Tata Mc Graw-Hill Publishing Company Limited, New Delhi (1990).
4. "*Spectroscopy*", P.S. Kalsi, Wiley Eastern Ltd., New Delhi, Hyd., (1998).
5. "*Spectroscopy*", Jag Mohan, Narosa Publishing House, New Delhi (2000).
6. "*Nuclear Magnetic Resonance Spectroscopy*", Mala Datta, Sarup & Sons, New Delhi (2000).
- 7) "*Spectroscopy*" by William Kemp.
- 8) "*Spectroscopy*", Pavia, Lampman, Kriz & Vyvyan, Cengage Learning India Pvt. Ltd., New Delhi (2008).
- 9) "*Molecular Spectroscopy - Principles and Chemical Applications*", P.R. Singh and S.K. Dikshit, S. Chand & Co., New Delhi (1988).
- 10) "*Mass Spectroscopy*", Howe, Williams and Brown, Tata Mc Graw-Hill Publishing Company Limited, New Delhi (1990).
- 11) "*Organic Structures from Spectra*", L.D. Field, S. Sternhell and J.R. Kalman, John Wiley & Sons, New York (2002).
- 12). "*Nuclear Magnetic Resonance- Basic Principal*", Atta-ur- Rahman, Springer(India) Pvt. Ltd., New Delhi (2008).
- 13). "*Molecular Structure and Spectroscopy*", G. Aruldas, Eastern Economy Edition, 2nd Edition, New Delhi (2008).
- 14). "*Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR*", D.N. Sathyanarayana, I.K. Internataional Publishing House Pvt. Ltd., New Delhi (2009).
- 15). "*Fundamentals of Atomic & Molecular Spectroscopy*", Ramphal Sharma, Himalaya Publishing House Ltd., 1st Edition, New Delhi (2008).