CH E 516: ANALYTICAL AND GREEN CHEMISTRY

Course Outcome

- Enable the students to understand the basic principles and theory of UV/Electronic, Infra-Red, Nuclear Magnetic Resonance and Mass Spectroscopy.
- Study the utility of these techniques in structure elucidation of simple organic molecules.
- Know about water cycle, water sources, water quality, and significant measurements of water parameters and treatment of water for drinking and industrial purposes.
- Learn about principles and use of green chemistry in laboratory synthesis.
- Understand the green chemistry principles, basic principles and utility of sonochemistry and Microwave induced organic synthesis.

UNIT-I **[12 Hours]**

UV/Electronic Spectroscopy: Basic principles, Beer-Lambert law, types of absorption bands, Factors affecting the positions of UV bands. Theoretical prediction of λmax for polyenes, α,β-unsaturated aldehydes, ketones (Woodward-Fieser rules) and substituted benzenes.

IR Spectroscopy: Basic principles, Application of infrared spectroscopy in the structural study-identity by fingerprinting and identification of functional groups. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities.

Nuclear Magnetic Resonance Spectroscopy: Basic principles, Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spincoupling, coupling constant. Shielding and deshielding. High resolution ^{1}HNMR. Applications of NMR spectroscopy in structure elucidation of simple organic molecules.

Mass Spectrometry: Basic principles, molecular ions, meta-stable ions and isotope ions. Fragmentation processes, McLafferty rearrangement, retro Diels-Alder fragmentations. Nitrogen rule.

UNIT-II **[12 Hours]**

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality- safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques.

Determination and significance of DO, BOD, COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis. Treatment of liquid radioactive wastes.

UNIT-III **[12 Hours]**

Green Chemistry: Definition and principles, planning a green synthesis in a chemical laboratory, Green preparation-Aqueous phase reactions, solid state (solventless) reactions, photochemical reactions, Phase transfer catalyst catalysed reactions (Quaternary ammonium salts & Crown ethers), enzymatic transformations & reactions in ionic liquids.

Sonochemistry: Introduction, instrumentation, the phenomenon of cavitation, Sonochemical esterification, substitution, addition, oxidation, reduction and coupling reactions.

Microwave induced organic synthesis: Introduction, reaction vessel and reaction medium, concept, specific effect, atom efficiency, % atom utilisation, advantages and limitations, alkylation

of active methylene compounds, N-alkylation, condensation of active methylene compounds with aldehydes, Diels-Alder reaction, Leuckardt reductive amination of ketones, orthoester Claisen rearrangement.

References

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12. Organic Synthesis, Special Techniques, V. K. Ahluwalia and R. Aggarwal, Narosa (2001).
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