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| **logoUniversity of Management & Technology**  School of Science  **Department of Chemistry** |
| MS CHE-658: Spectroscopic Studies of Organic Molecules  Credit Hours 3 |

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| **Week** | **Course Outlines** |
| 1 | Introduction to electromagnetic radiations and spectroscopy, Spectroscopic techniques for organic molecules in research and industry, Molecular energy levels, Absorption of radiations/interaction with radiations, UV-Vis absorption spectroscopy, Electronic transitions, Instrumentation and spectrum recording. |
| 2 | UV-Vis Spectrum. Beer Lambert Law, Solvent effect, Conjugation and chromophore, Polyenes, Carbonyl compounds, Aromatic systems, Heterocyclic compounds, Modern applications of UV-Vis spectroscopy. |
| 3 | Infrared Spectroscopy, Molecular vibrations and their frequency calculations, Instrumentation- Dispersive IR, FTIR, Interpretation of IR spectra. |
| 4 | Functional groups characterization and frequency shift related to structural changes, IR radiations and greenhouse effect, Applications of IR spectroscopy |
| 5 | Introduction to NMR, Magnetic Field, shielding and deshielding in 1HNMR, spin-spin coupling, Splitting of NMR signals (n+1) rule, identification of location, intensity and splitting of proton signals |
| 6 | Adjacent and germinal protons coupling, Coupling Constants, Complex Splitting, identification of stereochemically nonequivalent proton, Anisotropic effect, Proton Spin Decoupling |
| 7 | Nuclear overhauser effect, Factors affecting chemical shifts, Spin-spin coupling to 13C |
| 8 | Advance NMR, 2D NMR Spectroscopy, Correlation spectroscopy, HMBC, HSQC, COSY, NOESY, EXSY, Quantitative applications |
| 9 | Combined NMR techniques- Practice Problems |
| 10 | Mass spectrometry (MS), various analyzers and sources for ionization of molecule, Instrumentation, DBR rule, Isotope methods |
| 11 | Fragmentation pattern to interpret spectra, Fragmentation in Ethers, sulfides, amines, aldehydes and ketones |
| 12 | Fragmentation pattern of carboxylic acid, amides, nitriles, nitro compounds and halides, Common fragment peaks, Common lost peaks |
| 13 | Gas Chromatography -Mass Spectrometry (GC-MS) of organic compounds |
| 14 | Practice in spectral analysis and structure determination of organic compounds |
| 15 | Practice in structure determination, Problems using a combination of spectroscopic techniques |