**School of Chemical Sciences**

**Devi Ahilya Vishwavidyalaya, Indore**

**M.Sc. Chemistry**

**SEMESTER III**

**MCH-301: MOLECULAR SPECTROSCOPY**

**Credits 3**

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| **Unit I** | Ultraviolet and Visible spectroscopy: Fundamentals, effect of solvent and extending conjugation on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic compounds. Steric effect in biphenyls  |
| **Unit II** | Nuclear Magnetic Resonance Spectroscopy-: Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant ‘J’ Classification of spin systems,(AXB, AMX, ABC, A2B2 etc.). First-order and Second-order spectra Basic idea about instrument, FT NMR, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), spin decoupling(double resonance), chemical exchange, effect of deuteration, stereochemistry, hindered rotation, NMR shift reagents, Solvent effect, Nuclear Overhauser effect (NOE).  |
| **Unit III** | Carbon-13 NMR Spectroscopy: General considerations, chemical shift (aliphatic olefinic , alkyne, aromatic, heteroaromatic and carboynl carbon), NMR studies of nuclei other than proton and carbon-19F and 31P.Two dimensional NMR spectroscopy: COSY, HETCOR, NOESY, DEPT,HMBC and HMQC techniques |
| **Unit IV** | Mass Spectrometry : Introduction, ion production EI, CI, FD, ESI and FAB, ion analysis, ion abundance, Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable ion peak, Mc Lafferty rearrangement , Nitrogen rule, High resolution mass spectrometry.Combined problems based on UV, IR, NMR and Mass spectral techniques |
|  | **Books Suggested**1. R.M. Silverstein, G.C. Bassler and T.C. Morrill, Spectrometric Identification of Organic Compounds, John Wiley
2. R.J. Abraham, J. Fisher and P. Loftus, Introduction to NMR spectroscopy, Wiley
3. J.R. Dyer, Application of Spectroscopy of Organic Compounds, Prentice Hall
4. D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw-Hill
5. Banwell, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill
6. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall
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