

# Test 1 Topic Summary – Chapters 12-14

## Chapter 12: Mass Spectrometry and Infrared Spectroscopy

- Uses of Mass Spec (obtaining molecular formula, fragmentation patterns)
- Use of IR to determine functional groups

## Chapter 13: Nuclear Magnetic Resonance Spectroscopy

- Four pieces of info from  $^1\text{H}$  NMR:
  - 1) Number of types of H (# of signals)
  - 2) Number of each type of H (integration)
  - 3) Number of neighboring H (coupling patterns – N+1 rule)
  - 4) Electronic environment of each type of H (chemical shift – how deshielded)
- $^{13}\text{C}$  NMR – including DEPT experiments (determines H substitution on C)
- Determining molecular structure from spectroscopic data

## Chapter 14: Conjugated Dienes and Ultraviolet Spectroscopy

- Conjugated diene - two C=C separated by one C–C
- Stability (orbital overlap, molecular orbitals)
- Electrophilic Additions to conjugated dienes – 1,2 and 1,4 addition
- Allylic carbocation stability
- Kinetic (cold) vs. Thermodynamic (hot) control
- Diels-Alder reactions – good dienophiles, stereoselectivity (endo)
- $\text{S}_{\text{N}}2'$  - front side side attack
- UV Spectroscopy ( $\pi \rightarrow \pi^*$ )