

IR Spectroscopy

around 3000 cm^{-1}

to left, broad

to left, sharp

to right

OH or NH

sp^2 or sp CH

sp^3 CH

around 1700 cm^{-1}

to left ($1700-1800\text{ cm}^{-1}$)

C=O

to right ($1600-1680\text{ cm}^{-1}$)

C=C

between 1700 and 3000 cm^{-1}

$\sim 2200\text{ cm}^{-1}$

$\text{C}\equiv\text{C}$ or $\text{C}\equiv\text{N}$

(know that can use CH cop to tell sub-pattern of alkene ($1000-600\text{ cm}^{-1}$))

^1H NMR Spectroscopy

0-2.5 ppm

sp^3 CH's

2.5-5.0 ppm

H-C-A (A is a heteroatom)

5.0-6.0 ppm

H=C=C

6.0-8.0 ppm

H-aromatic

past 9.0 ppm

$\frac{1}{2}$ $\overset{\text{O}}{\parallel}\text{C}$ H (sharp) or $\overset{\text{O}}{\parallel}\text{C}$ OH (broad)

H's on O or N usually broad, 1-5 ppm, can be absent
splitting (n+1) / integration

^{13}C NMR Spectroscopy

0-60 ppm

sp^3 C

60-100 ppm

C-A

100-165 ppm

$\overset{\text{O}}{\parallel}\text{C}$ sp^2 C (both alkene & aromatic)

165-200 ppm

$\overset{\text{O}}{\parallel}\text{C}$ or $\overset{\text{O}}{\parallel}\text{C}$ H

past 200 ppm

using unsaturation number (determined from molecular formula)

$$U = \frac{(2 \times \text{number of C} + 2) - (\text{number of H})}{2}$$

for halogen, count as a hydrogen
for oxygen, ignore it
for each N, subtract 1 hydrogen