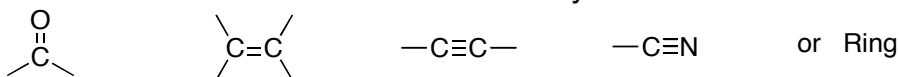


# Structure Determination Strategy

## I. IDENTIFY COMPONENTS:

### A. Molecular Formula: Determine/ identify IHD



### B. C-13 NMR

Identify Components

Identify symmetry

Proton inventory (formulae with heteroatoms)

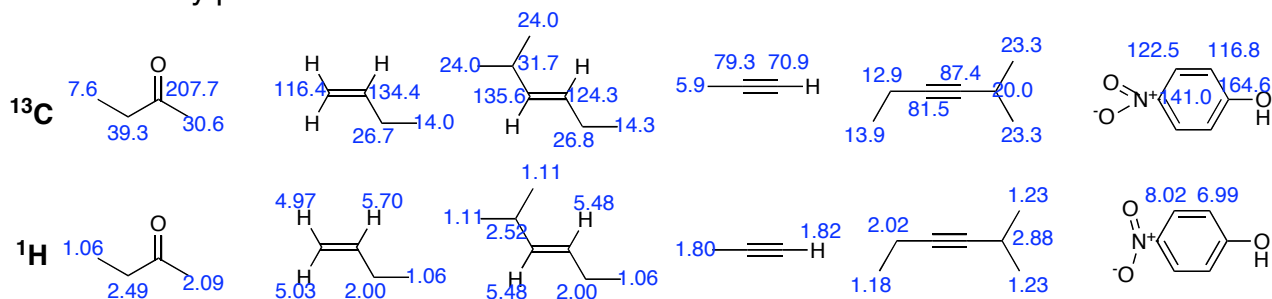
### C. IR, if available: (Functional group identification)

## II. CONNECT COMPONENTS:

### A. Explore around functional groups:

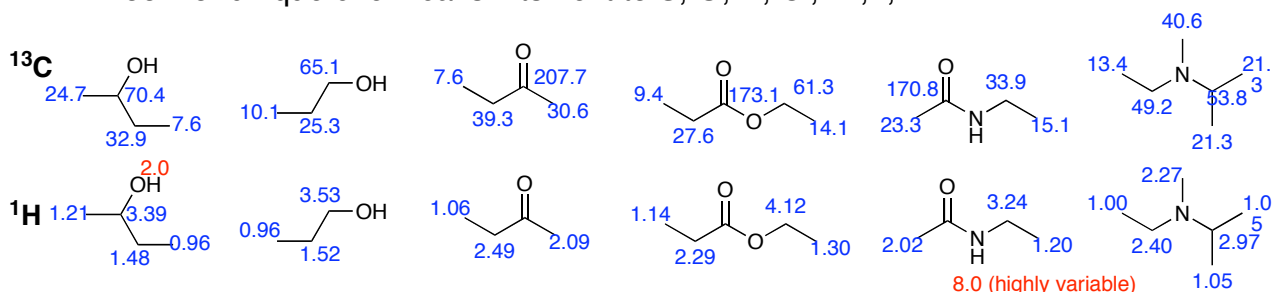
#### 1. Multiple bonds

Look for unique chemical shifts next to C=O, C=C and aromatics  
identify peaks in  $^1\text{H}$  and  $^{13}\text{C}$  NMR:

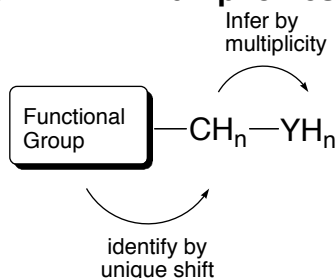


#### 2. Heteroatoms

Look for unique chemical shifts next to S, O, N, Cl, Br, I, F...



### B. Use $^1\text{H}$ -NMR multiplicities to infer adjacent groups.



### C. Isolated functional groups and substitutions on conjugated systems

1. MS: predict fragmentations based on functional groups

2. UV. Identify conjugated systems.