

Solving Combined Spectra Problems:

Mass Spectra:

Molecular Formula

Nitrogen Rule # of nitrogen atoms in the molecule

M+1 peak # of carbons

Degrees of Unsaturation: # of rings and/or π -bonds

Infrared Spectra

Functional Groups

C=O

C=C

C C

^1H NMR:

Chemical Shift (δ) chemical environment of the H's

Integration # of H's giving rise to the resonance

Spin-Spin Coupling (multiplicity) # of non-equivalent H's on the adjacent carbons (vicinal coupling).

Schoolery's Rules: final check on the structure assignment by ^1H NMR

^{13}C NMR

of resonances symmetry of carbon framework

Type of Carbonyl

Each piece of evidence gives a fragment (puzzle piece) of the structure. Piece the puzzle together to give a proposed structure. The proposed structure should be consistent with all the evidence.