

CONCEPT: STRUCTURE DETERMINATION – MOLECULAR SENTENCES

The holy grail of this section is **structure determination**.

- You may be asked to produce a structure from scratch given only a MF, NMR Spectrum and IR Spectrum.
- Our goal is to build a strong “molecular sentence” by gathering clues, then propose drawings.

How to build a molecular sentence:

1. Determine IHD.
2. Analyze NMR, IR and splitting patterns, integrations for major clues (i.e.).
 - NMR = 9.1 ppm _____
 - IR = 1710 cm⁻¹ _____
 - Triplet/Quartet _____
 - 9.1 ppm (2H) _____
3. Calculate ¹H NMR Signal : Carbon Ratio.
 - Ratio < ½ suggests symmetrical, whereas ratio > ½ suggests asymmetrical
 - Never rule out a structure based on symmetry (you may not be able to visualize it)
4. State the number of ¹H NMR signals needed.

--- DRAW POSSIBLE STRUCTURES ---

5. Use a combination of Shifts, Integrations, and Splitting to **confirm** which structure is correct.

EXAMPLE: Build a strong molecular sentence using the following data.

MF: C₄H₆O₂

IR: peak at 2950 cm⁻¹
peak at 2700 cm⁻¹
peak at 1720 cm⁻¹

¹H NMR
- 2.2 (doublet, 4H)
- 9.4 (triplet, 2H)

PRACTICE: Propose a structure for the following compound that fits the following ^1H NMR data:

Formula: $\text{C}_3\text{H}_8\text{O}_2$

^1H NMR: 3.36 δ (6H, singlet)

4.57 δ (2H, singlet)

PRACTICE: Propose a structure for the following compound that fits the following ^1H NMR data:

Formula: $\text{C}_2\text{H}_4\text{O}_2$

^1H NMR: 2.1 δ (singlet, 1.2 cm)

11.5 δ (0.5 cm, D_2O exchange)

PRACTICE: Propose a structure for the following compound that fits the following ^1H NMR data:

Formula: $\text{C}_{10}\text{H}_{14}$

^1H NMR: 1.2 ppm (6H, doublet)

2.3 ppm (3H, singlet)

2.9 ppm (1H, septet)

7.0 ppm (4H, doublet)

PRACTICE: Propose a structure for the following compound, $C_7H_{12}O_2$ with the given ^{13}C NMR spectral data:

Broadband decoupled ^{13}C NMR: 19.1, 28.0, 70.5, 129.0, 129.8, 165.78 δ

DEPT-90: 28.0, 129.8 δ

DEPT-135: 19.1 δ (\uparrow), 28.0 (\uparrow), 129.8 δ (\uparrow), 70.5 δ (\downarrow) & 129.0 δ (\downarrow)

PRACTICE: Propose a structure for the following compound, C₅H₁₀O with the given ¹³C NMR spectral data:

Fully Broadband decoupled ¹³C NMR and DEPT: 206.0 δ (↑); 55.0 δ (↑); 21.0 δ (↓) & 11.0 δ (↑).

PRACTICE: Provide the structure of the unknown compound from the given information.

Formula: $\text{C}_4\text{H}_{10}\text{O}$

IR: $3200\text{--}3600\text{ cm}^{-1}$

^1H NMR: 0.9 ppm (6H, doublet)

1.8 ppm (1H, nonatet)

2.4 ppm (1H, singlet)

3.3 ppm (2H, doublet)

PRACTICE: Provide the structure of the unknown compound from the given information.

Formula: $\text{C}_4\text{H}_9\text{N}$

IR: 2950 cm^{-1} , 3400 cm^{-1}

^1H NMR: 1.0 ppm (4H, triplet)

2.1 ppm (4H, triplet)

3.2 ppm (1H, singlet)