Spectral problem 1

\[ C_7H_{14}O \]

\[ ^{13}\text{C-NMR}: \delta 22.1, 25.4, 28.9, 58.3, 207.1. \]
Spectral Problem 1: answer

- **Formula:**
  one unsaturation

- **$^{13}\text{C NMR:}$**
  5 kinds of carbon
  Carbonyl group ($\delta$ 207)
  - The unsaturation!

- **$^{1}\text{H NMR:}$**
  3 kinds of hydrogen
  2H and 3H next to the carbonyl ($\delta$ 2.0-2.5)
  9 equivalent hydrogen: tert-butyl group!
Spectral problem 2

$\text{C}_4\text{H}_{10}\text{O}$
Spectral Problem 2: answer

- **Formula:**
  Fully saturated, with 4 carbon atoms

- **IR:**
  Alcohol

- **$^{13}$C NMR:**
  4 kinds of carbon

- **$^1$H NMR:**
  Integration: ~1:10 (since there are 10 H, 1:9)
  1H peak at 3.8: geminal to oxygen

- Only one $C_4H_{10}O$ alcohol isomer with 4 kinds of carbon and a single hydrogen geminal to oxygen!
Spectral problem 3: MS

MASS SPECTRUM

Rel. Abundance

m/z

0.  20.  40.  60.  80.  100.

0.  20.  40.  60.  80.  100.

27  41  56  84
Spectral problem 3: MS interpretation

- Molecular ion: 84
  Possible formulas: $C_6H_{12}$, $C_5H_8O$, $C_4H_4O_2$, $C_4H_8N_2$
- Base peak: 56 (M-28)
  28 is $C_2H_4$, $CH_2N$, or $CO$
  $C_2H_4$ is most likely
Spectral problem 3: IR/NMR
Spectral Problem 3: answer

- **IR:**
  No multiple bonds; no OH or NH

- **NMR:**
  One kind of H, one kind of C: high symmetry
  Chemical shifts indicate no C-C multiple bonds and no electronegative groups (nitrogen or oxygen)

- **Formulas:**
  C₆H₁₂: only reasonable formula with no N or O
  C₆H₁₂: one point of unsaturation = ring
  Only one 6-C ring with only one kind of carbon!
Spectral problem 4: MS

MASS SPECTRUM

Rel. Abundance

m/z

0.  20.  40.  60.  80.  100.  120.

0.  20.  40.  60.  80.  100.  120.
Spectral problem 4: MS interpretation

- Molecular ion: 100
  \[ \text{C}_7\text{H}_{16}, \text{C}_6\text{H}_{12}\text{O}, \text{C}_5\text{H}_8\text{O}_2, \text{C}_5\text{H}_{10}\text{N}_2, \text{etc.} \]

- Only other large peaks: 59 and 41
  - 59: M - 41! \text{C}_4\text{H}_{11}^+ \text{ or C}_3\text{H}_7\text{O}^+ \text{ or C}_2\text{H}_3\text{O}_2^+
  - 41: \text{C}_3\text{H}_5^+ \text{ (allyl cation)}
Spectral problem 4: IR/NMR
Spectral Problem 4: answer

- **IR:**
  - C=O and C=C, but no OH

- **$^{13}$C NMR:**
  - 5 kinds of C: 2 saturated, 3 unsaturated
  - C=O is an ester ($\delta$ 169)
  - Saturated C-O ($\delta$ 51)

- **$^1$H NMR:**
  - 4 kinds of H: two vinylic, two methyl
  - Methyl group on O ($\delta$ 3.8)
  - Methyl group on C=C ($\delta$ 2.0)
  - No splitting of methyl peaks

- **Formulas:**
  - $\text{C}_5\text{H}_8\text{O}_2$ is only one with two oxygen, five carbon
Spectral problem 5: MS
Spectral problem 5: MS interpretation

- Molecular ion: 118
  Possible formulas: $C_9H_{10}$, $C_8H_6O$, $C_6H_{14}O_2$
- Base peak: 117
  Easy loss of one H; a number of functionalities (benzylic H, allyl H, aldehyde H are all easily lost from the molecular radical cation)
Spectral problem 5: IR/NMR

$^{13}$C NMR: 137.4, 128.4, 127.7, 126.2, 121.7, 16.6
Spectral Problem 5: answer

- **IR:**
  - No OH, C=O

- **$^{13}$C NMR:**
  - 6 kinds of C; only one is saturated

- **$^1$H NMR:**
  - 5 aromatic H
  - 2 vinylic H
  - 3 methyl H (doublet means next to 1 H)

- **Formula:**
  - Has to be $C_9H_{10}$; no other possible with 10 H