Assign peaks in the $^{13}\text{C}$ spectrum of ethyl benzoate.
Solution:

- $M^+ = 86 \rightarrow C_5H_{10}O$
- IR at 3400 cm$^{-1} \rightarrow$ alcohol
- $^{13}$C NMR: $\delta$ 30.2, 31.9, 61.8, 114.7, 138.4 shows an alkene
- DEPT-90: $\delta$ 138.4
- DEPT-135
  - Positive peak $\delta$ 138.4
  - Negative peaks $\delta$ 30.2, 31.9, 61.8, 114.7
  - Shows one CH (vinylic), four CH$_2$ (one vinylic)
Solution

- Isomeric with previous $\rightarrow$ C$_5$H$_{10}$O
- $^{13}$C NMR: $\delta$ 9.7, 29.9, 74.4, 114.4, 141.4 shows an alkene with one saturated C next to oxygen
- DEPT-90: $\delta$ 74.4, 141.4
- DEPT-135
  - Positive peaks $\delta$ 9.7, 74.4, 141.4
  - Negative peaks $\delta$ 29.9, 114.4
  - Shows two CH (one vinylic, one saturated & bonded to O), one CH$_3$, two CH$_2$ (one vinylic)
Solution to Problem 1

- **MS**: 44, 43, 29, 15
  - C\(_3\)H\(_8\), C\(_2\)H\(_4\)O
- **IR**: C=O at 1750 cm\(^{-1}\)
  - small, sharp peak at 3500 is the overtone!
- **\(^{13}\)C NMR**: 
  - CH at 200 is C=O
  - CH\(_3\) at 37 ppm
Solution to problem 2

**IR:**
- C=O at 1750 cm⁻¹

**MS:** M⁺=84
- C₆H₁₂; C₅H₈O

**¹³C NMR:**
- C=O at 220 is ketone
- CH₂ at 24, 41 ppm
- No methyl groups! Must be a ring
Solution to problem 3

- **$^{13}$C NMR:**
  - 7 kinds of carbon
  - Probably aromatic
- **MS:** $M^+ = 118$
  - $C_9H_{10}$; $C_8H_6O$??
  - 5 points of unsat.
- **NMR:**
  - 1 methyl group
  - 1 terminal vinyl
  - 3 kinds of $\text{CH}=(\text{c})$
  - 2 quaternary $\text{C}=(\text{c})$
Solution to problem 4

- **IR:** C=O
- **MS:** M^+ = 148
  - C\textsubscript{11}H\textsubscript{16}; C\textsubscript{10}H\textsubscript{12}O; etc.
- **\textsuperscript{13}C NMR:**
  - Aliphatic ketone at 205 ppm
  - Probable benzene ring (CH, C 120-142)
  - 3 saturated C: 2 CH\textsubscript{2}, 1 CH\textsubscript{3}