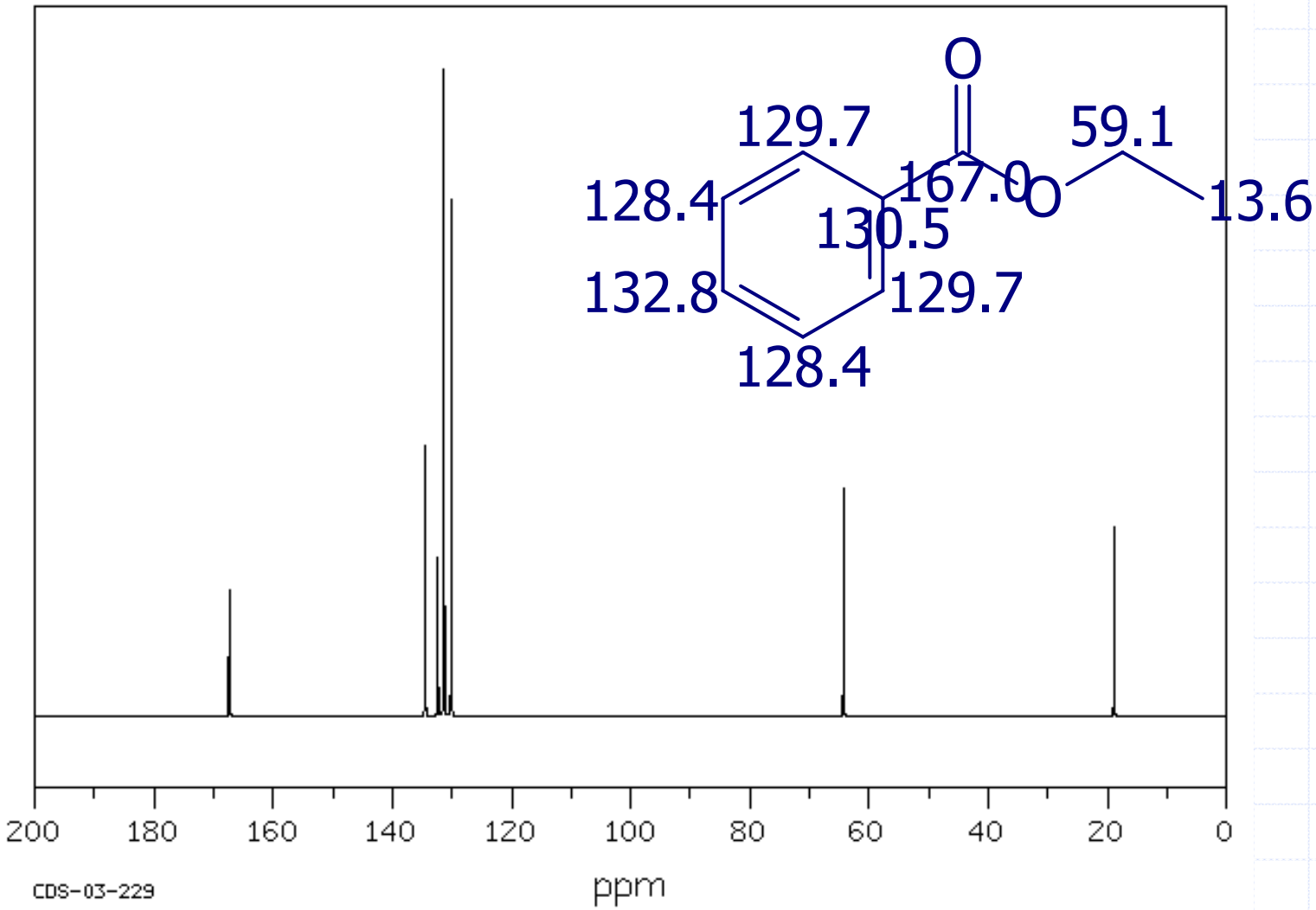
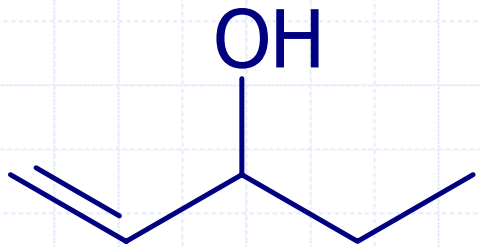
Assign peaks in the ^{13}C spectrum of ethyl benzoate

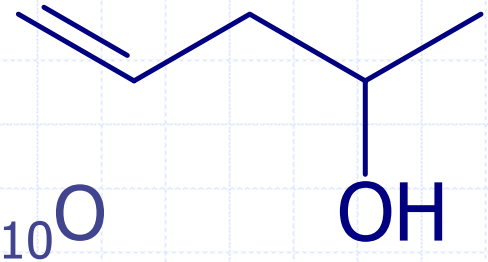


Solution:

- $M^+ = 86 \rightarrow C_5H_{10}O$
- IR at 3400 $cm^{-1} \rightarrow$ alcohol
- ^{13}C NMR: δ 30.2, 31.9, 61.8, 114.7, 138.4 shows an alkene
- DEPT-90: δ 138.4
- DEPT-135
  - Positive peak δ 138.4
  - Negative peaks δ 30.2, 31.9, 61.8, 114.7
  - Shows one CH (vinylic), four CH_2 (one vinylic)

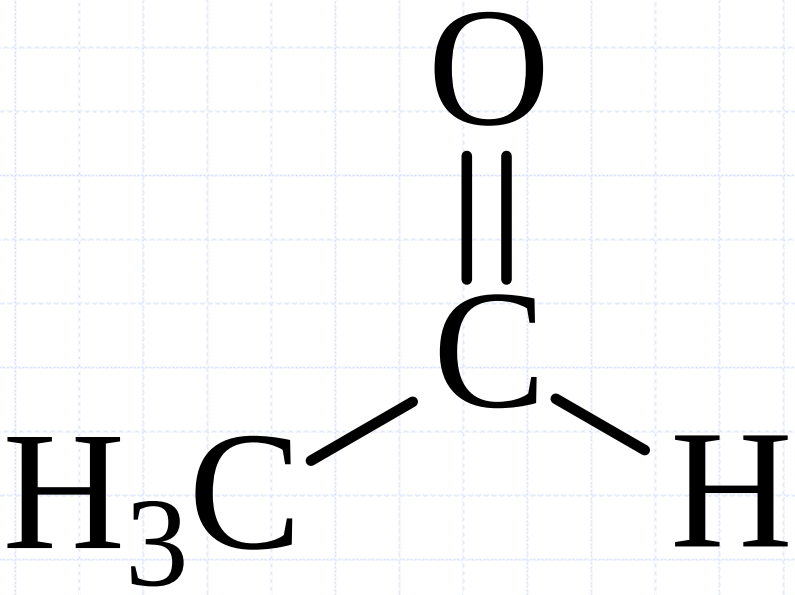
Solution





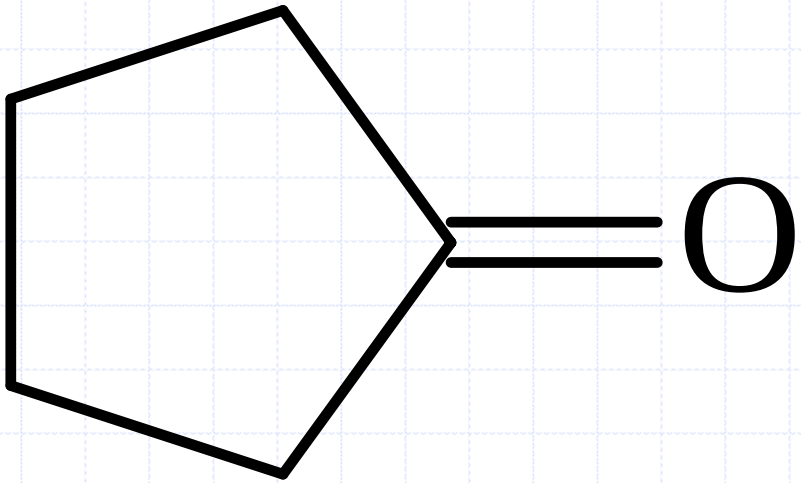
- Isomeric with previous → $C_5H_{10}O$
- ^{13}C NMR: δ 9.7, 29.9, 74.4, 114.4, 141.4 shows an alkene with one saturated C next to oxygen
- DEPT-90: δ 74.4, 141.4
- DEPT-135
  - Positive peaks δ 9.7, 74.4, 141.4
  - Negative peaks δ 29.9, 114.4
  - Shows two CH (one vinylic, one saturated & bonded to O), one CH_3, two CH_2 (one vinylic)

Solution to Problem 1



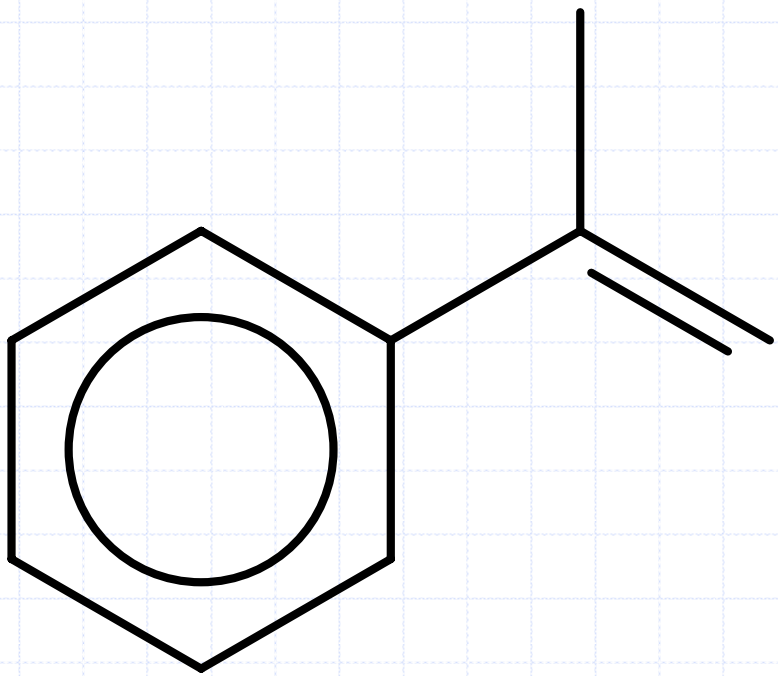
- MS: 44, 43, 29, 15
  - C_3H_8, C_2H_4O
- IR: C=O at 1750 cm^{-1}
  - small, sharp peak at 3500 is the overtone!
- ^{13}C NMR:
  - CH at 200 is C=O
  - CH_3 at 37 ppm

Solution to problem 2



- IR:
  - C=O at 1750 cm^{-1}
- MS: M^+=84
  - C_6H_{12}; **C_5H_8O**
- ^{13}C NMR:
  - C=O at 220 is ketone
  - CH_2 at 24, 41 ppm
  - No methyl groups! Must be a ring

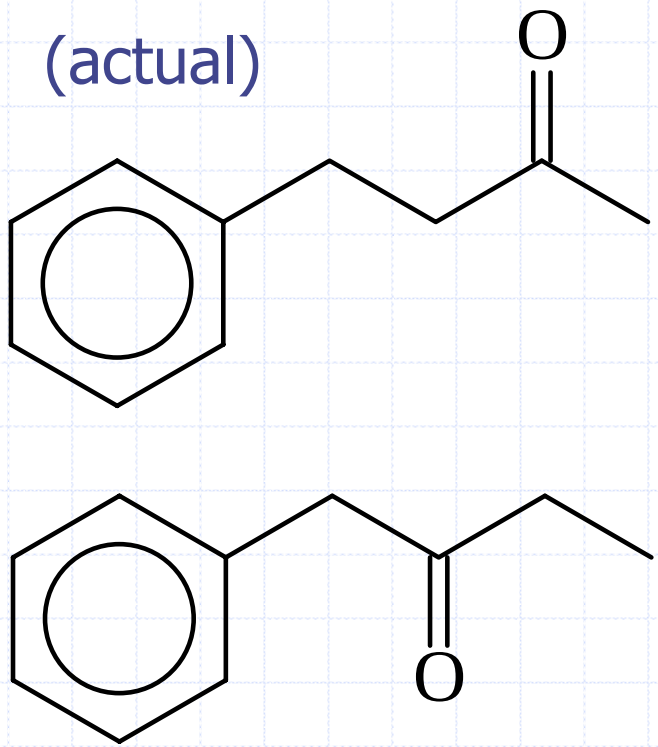
Solution to problem 3



- ^{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 CH=(c)
  - 2 quaternary C=(c)

Solution to problem 4

(actual)



- IR: C=O
- MS: M^+=148
  - $C_{11}H_{16}$; $C_{10}H_{12}O$; etc.
- ^{13}C NMR:
  - Aliphatic ketone at 205 ppm
  - Probable benzene ring (CH, C 120-142)
  - 3 saturated C
    - 2 CH_2, 1 CH_3