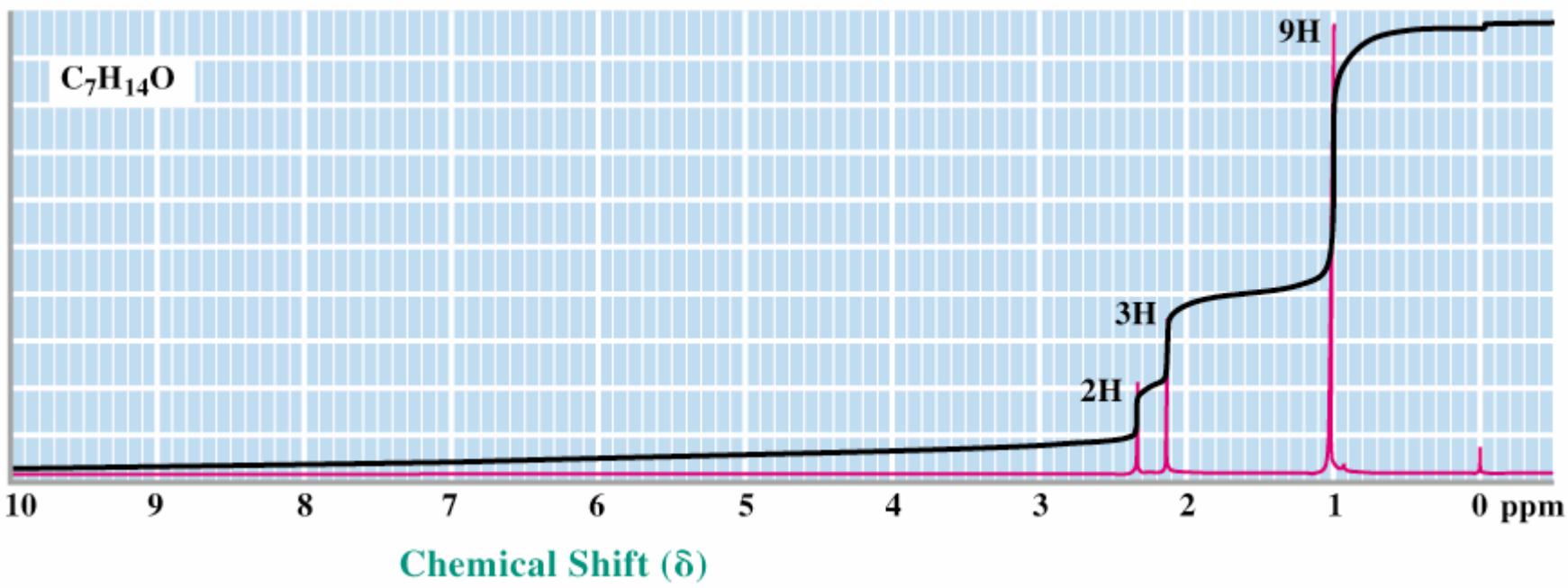
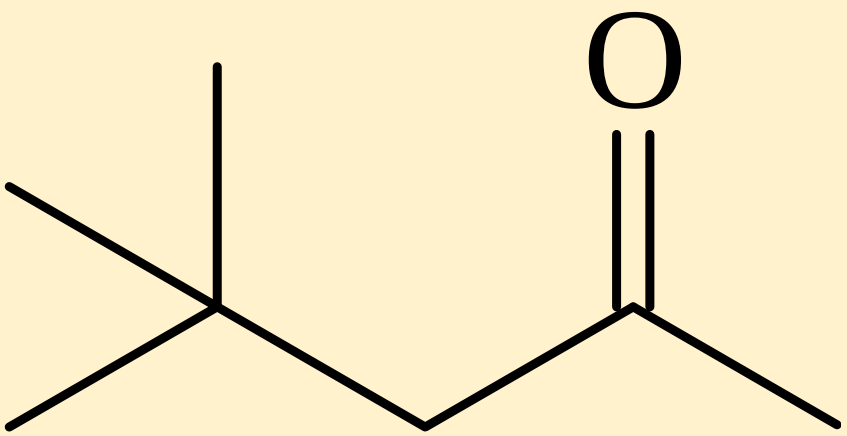
Spectral problem 1



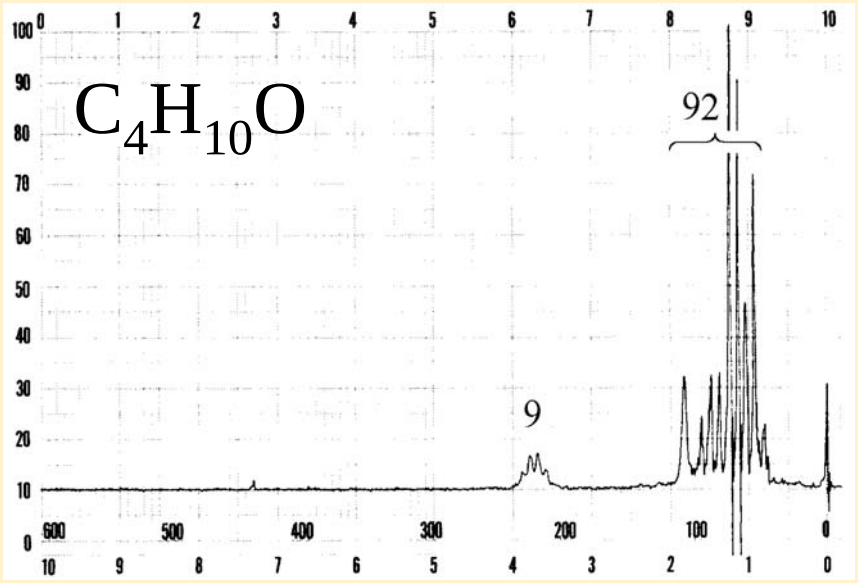
^{13}C-NMR: δ 22.1, 25.4, 28.9, 58.3, 207.1.

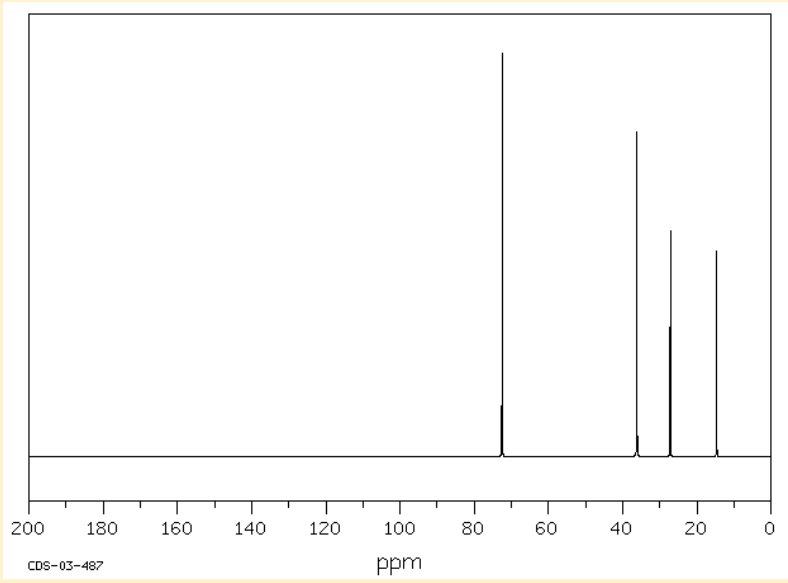
Spectral Problem 1: answer

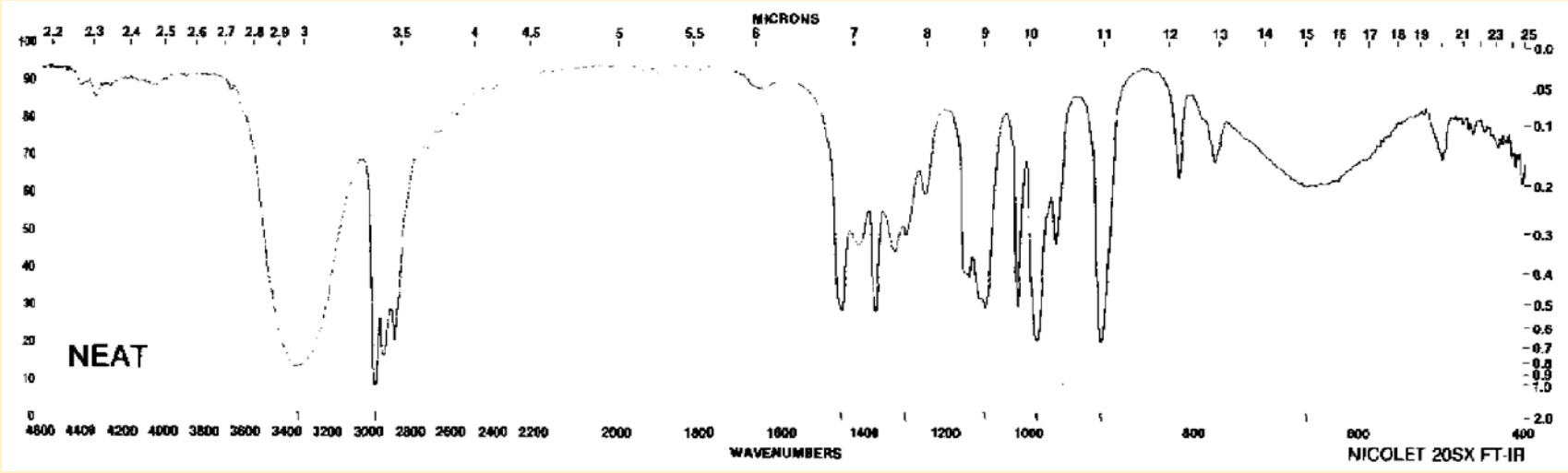


- **Formula:**
  - one unsaturation
- **^{13}C NMR:**
  - 5 kinds of carbon
  - Carbonyl group (δ 207)
    - **The unsaturation!**
- **^{1}H NMR:**
  - 3 kinds of hydrogen
  - 2H and 3H next to the carbonyl (δ 2.0-2.5)
  - 9 equivalent hydrogen: tert-butyl group!

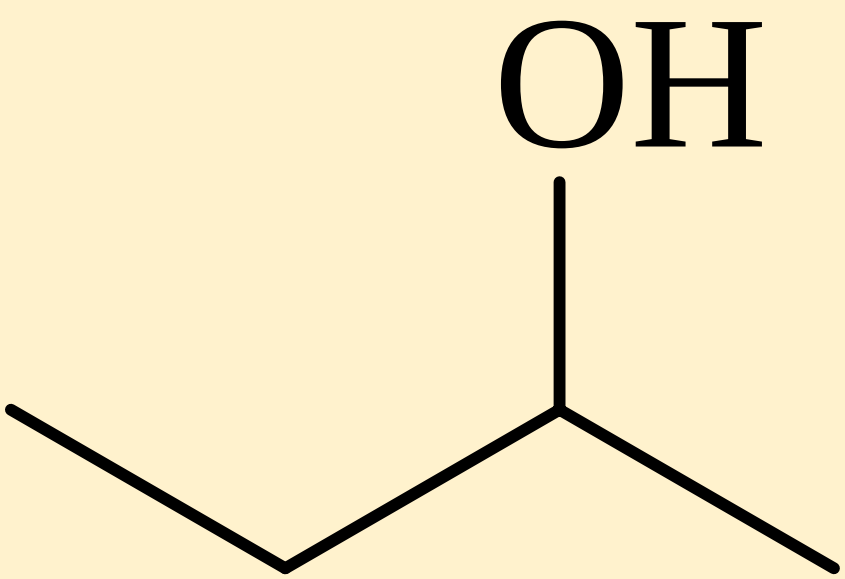
Spectral problem 2





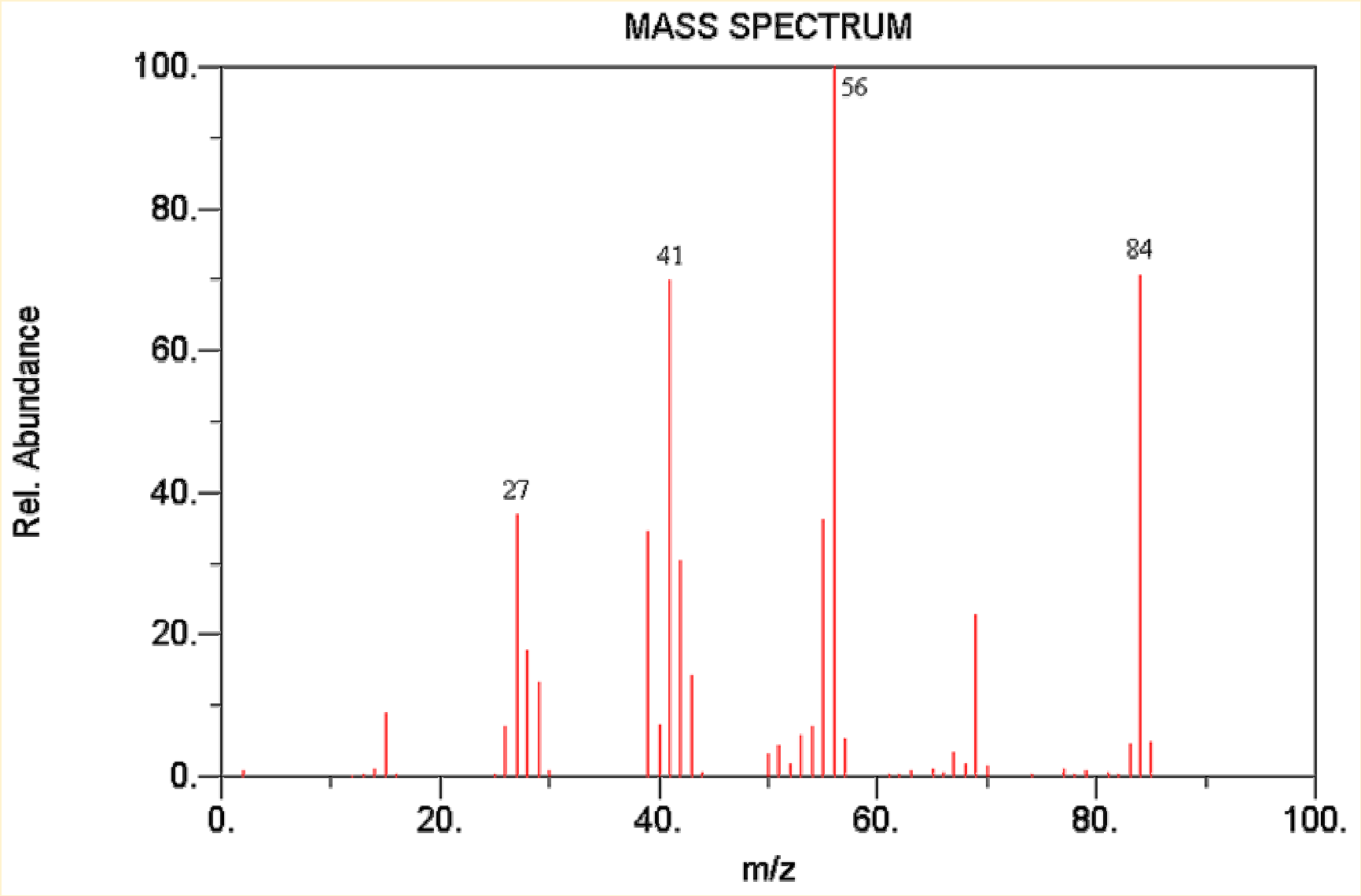


Spectral Problem 2: answer



- **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!**

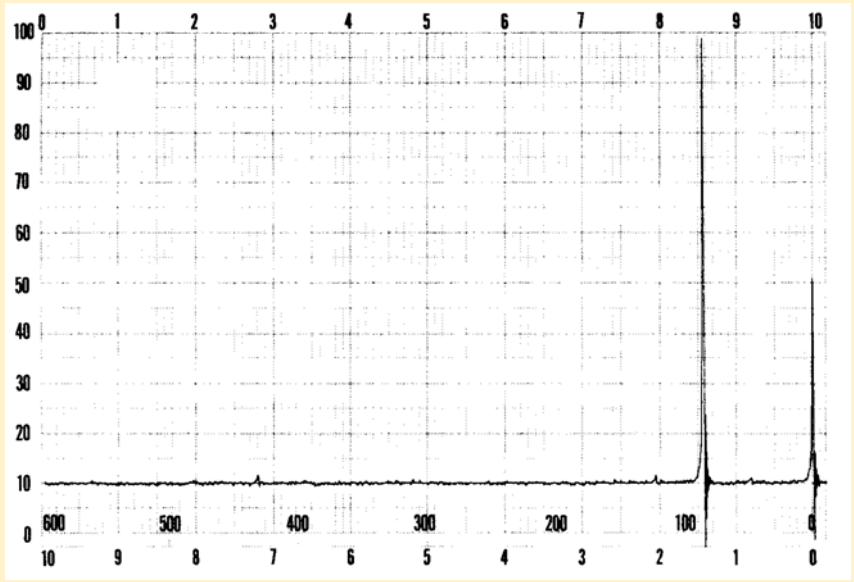
Spectral problem 3: MS

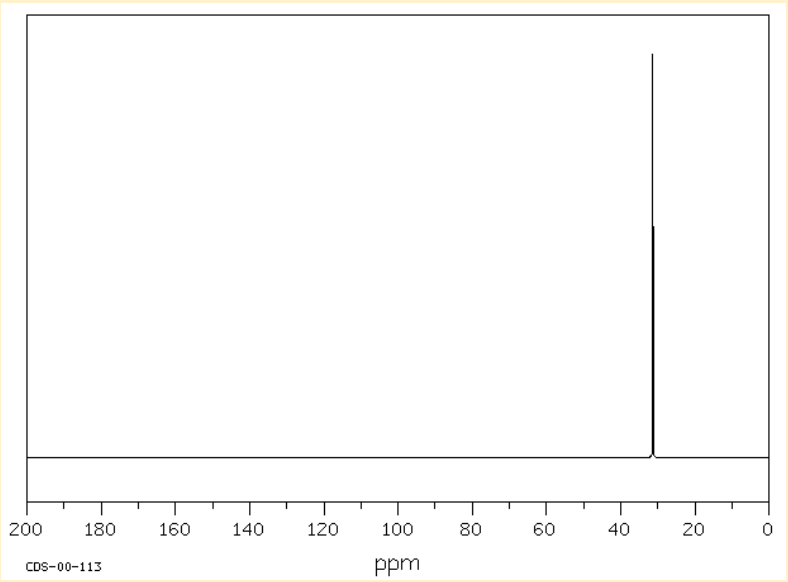


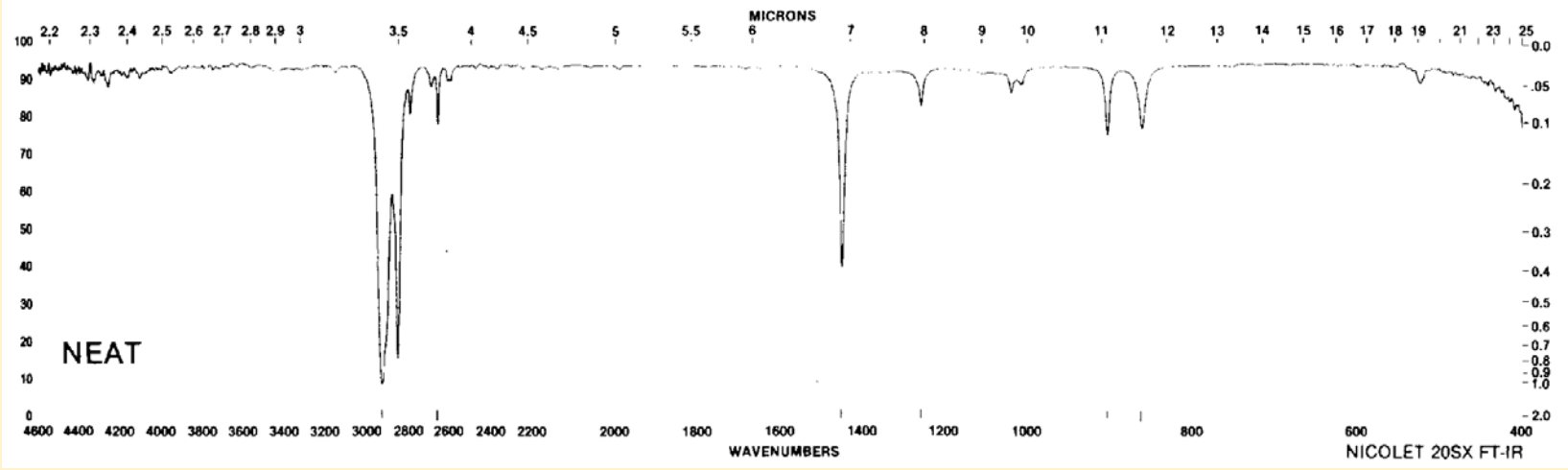
Spectral problem 3: MS interpretation

- **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

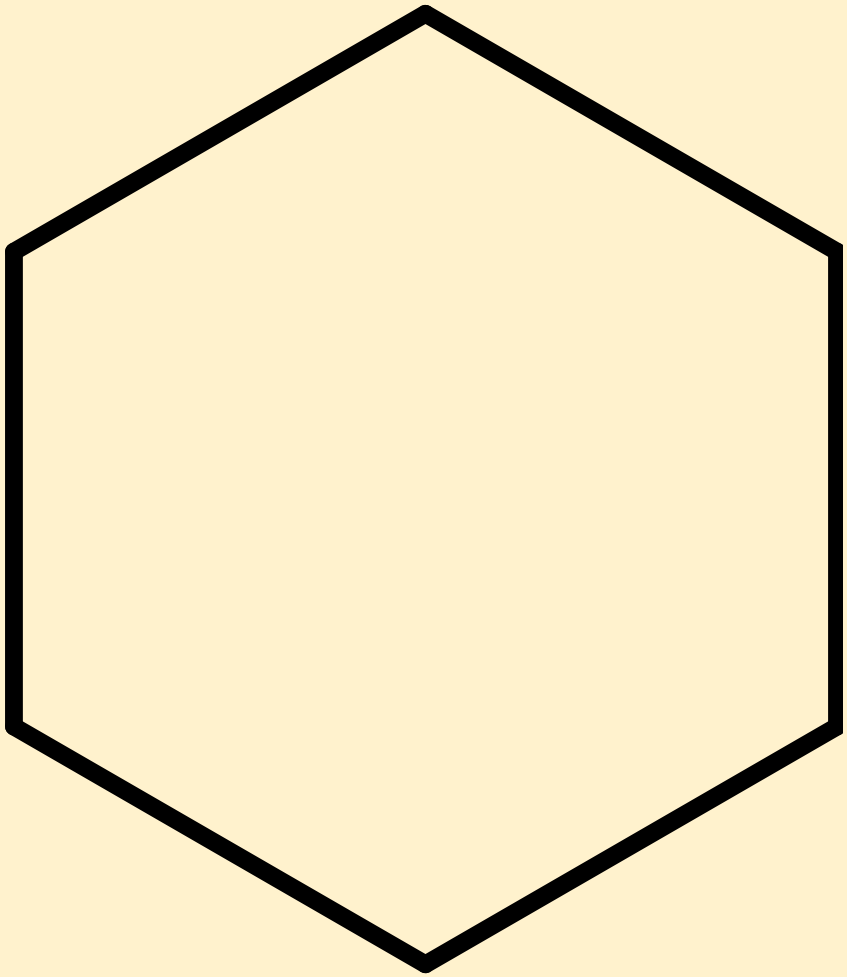
Spectral problem3: IR/NMR





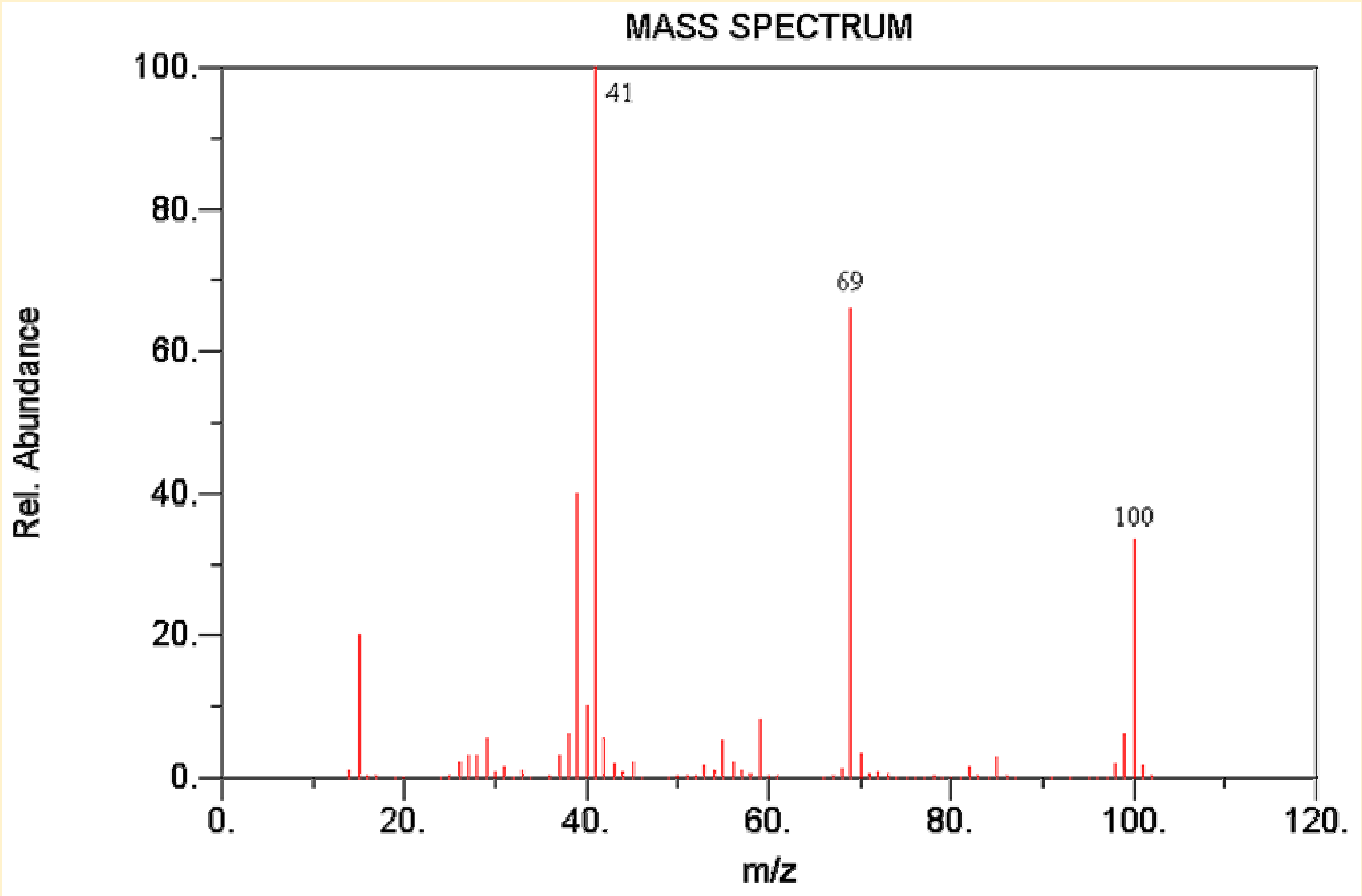


Spectral Problem 3: answer



- **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:**
  - C_6H_{12}: only reasonable formula with no N or O
  - C_6H_{12}: one point of unsaturation = ring
  - Only one 6-C ring with only one kind of carbon!

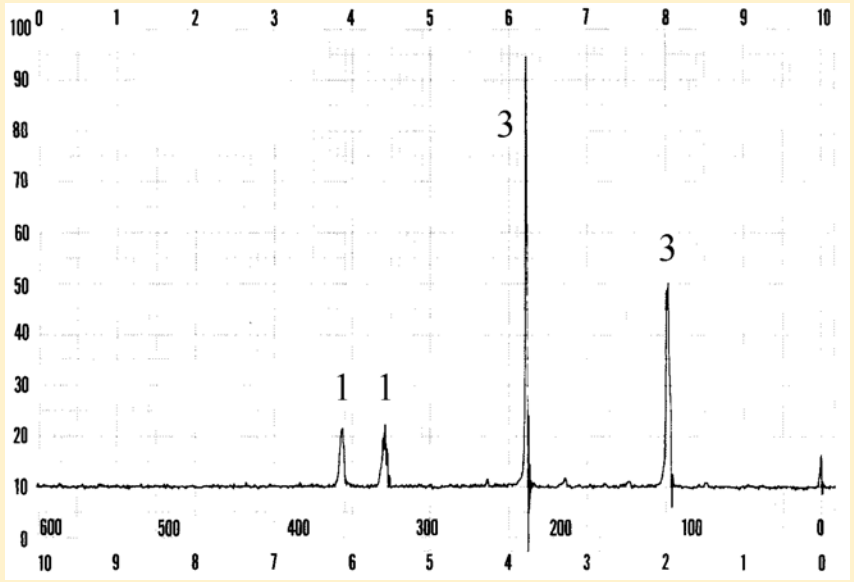
Spectral problem 4: MS

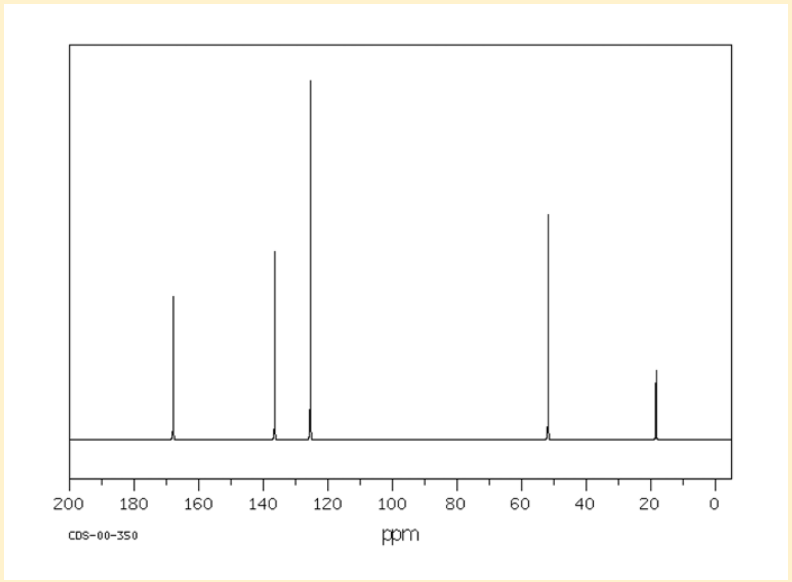


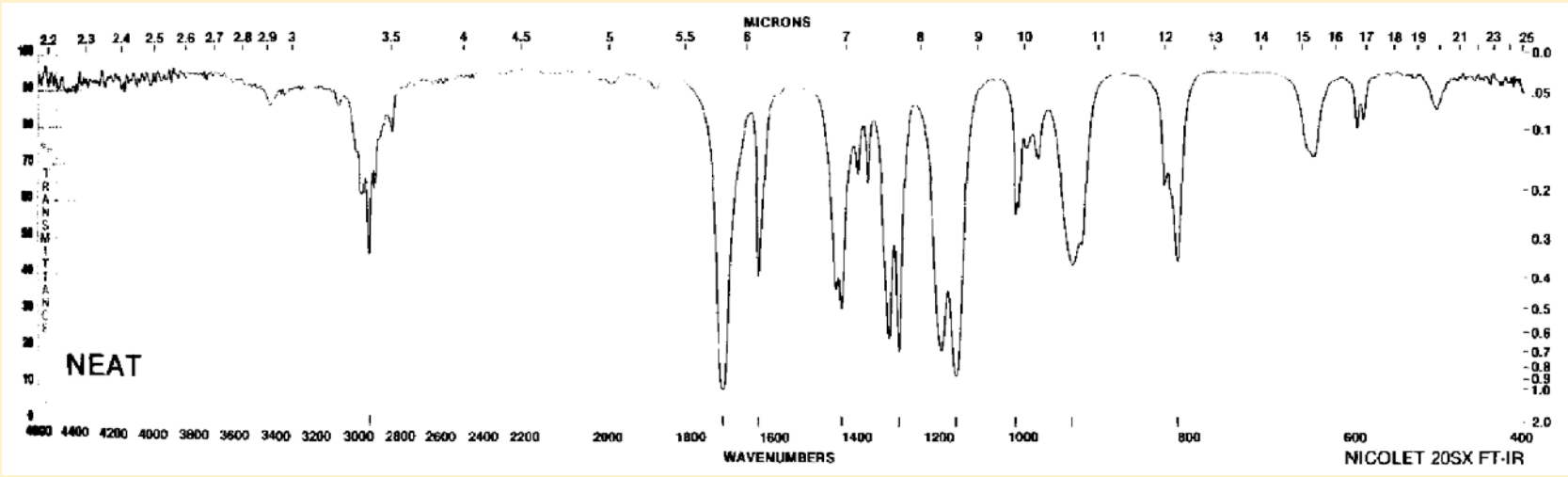
Spectral problem 4: MS interpretation

- **Molecular ion: 100**
  - C_7H_{16}, $C_6H_{12}O$, $C_5H_8O_2$, $C_5H_{10}N_2$, etc.
- **Only other large peaks: 59 and 41**
  - 59: M - 41! $C_4H_{11}^+$ or $C_3H_7O^+$ or $C_2H_3O_2^+$
  - 41: $C_3H_5^+$ (allyl cation)

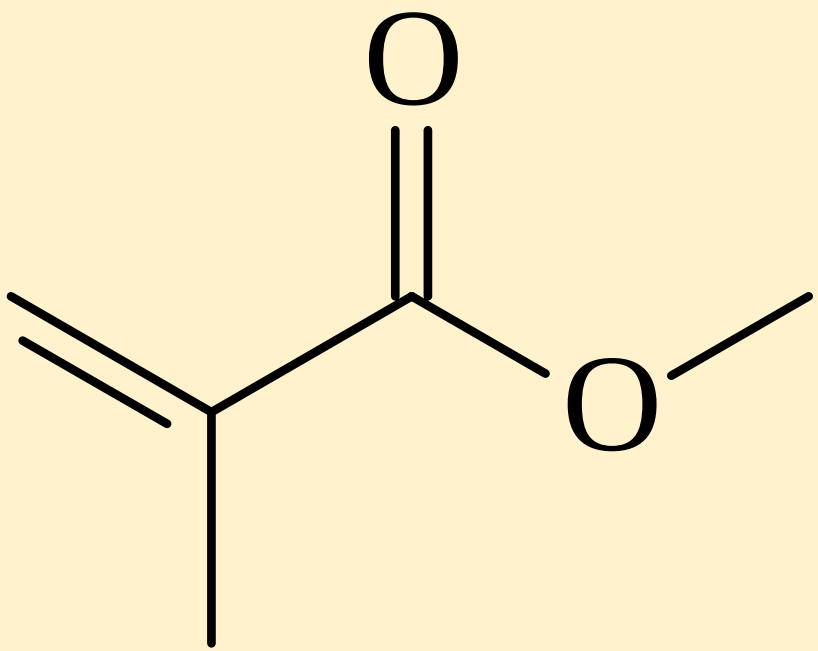
Spectral problem 4: IR/NMR





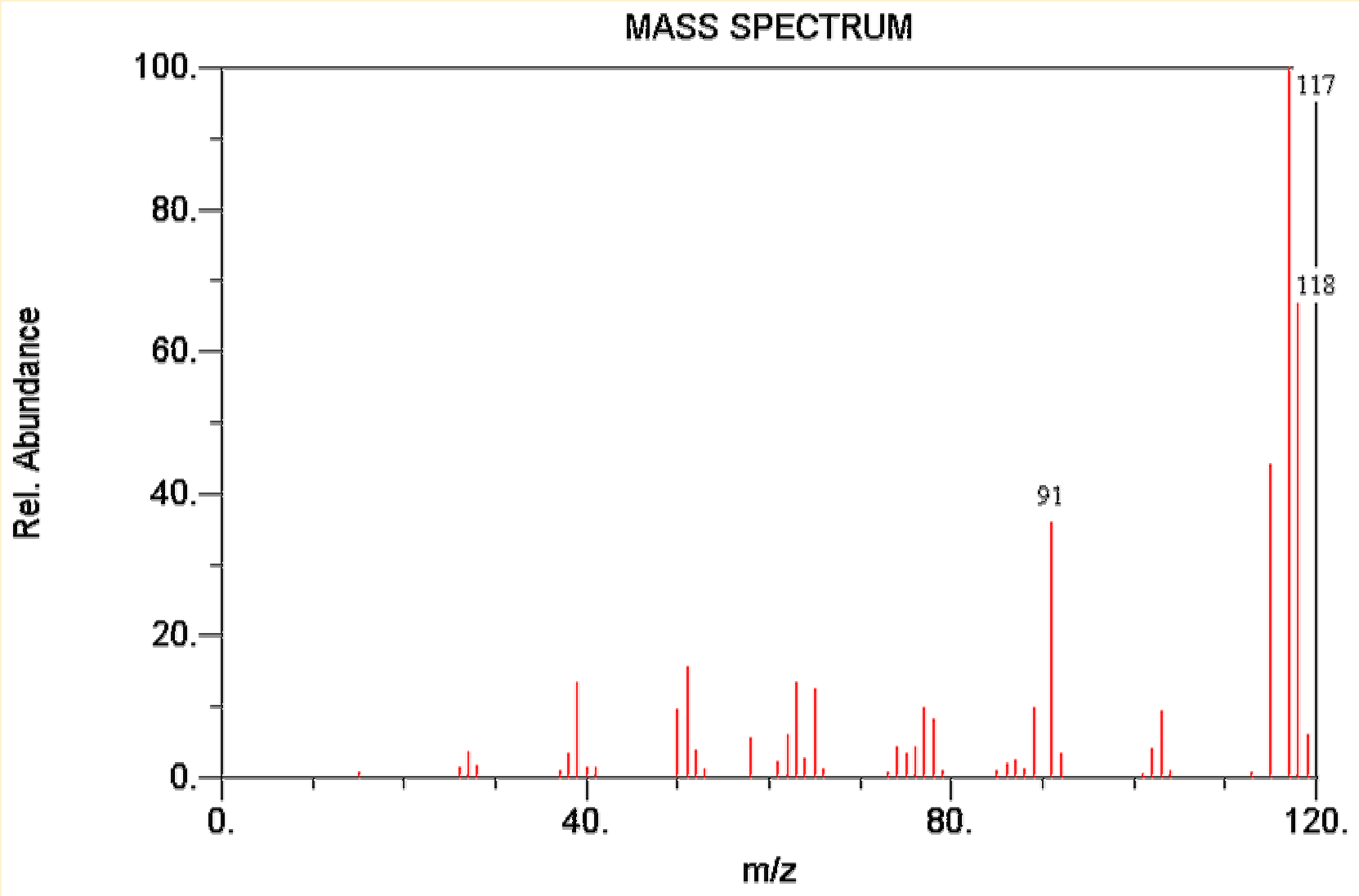


Spectral Problem 4: answer



- **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 (δ 169)
  - Saturated C-O (δ 51)
- **^{1}H NMR:**
  - 4 kinds of H: two vinylic, two methyl
  - Methyl group on O (δ 3.8)
  - Methyl group on C=C (δ 2.0)
  - No splitting of methyl peaks
- **Formulas:**
  - $C_5H_8O_2$ is only one with two oxygen, five carbon

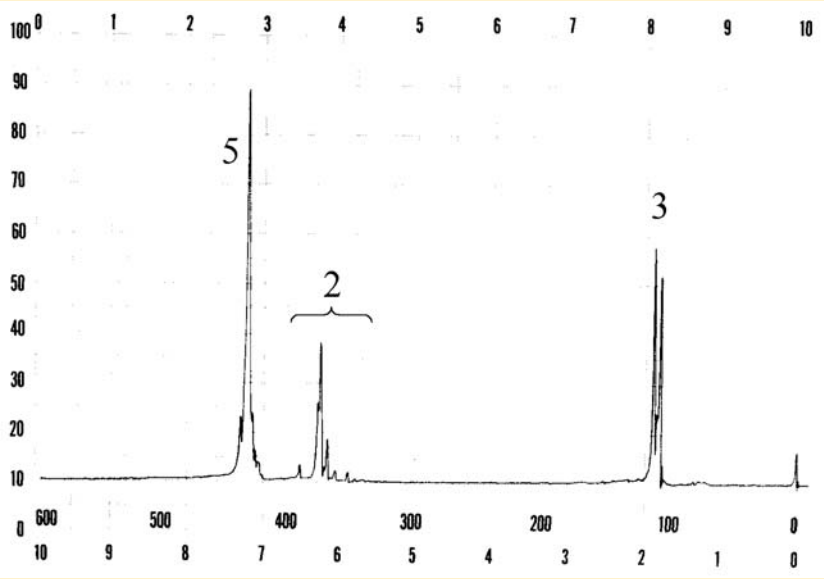
Spectral problem 5: MS



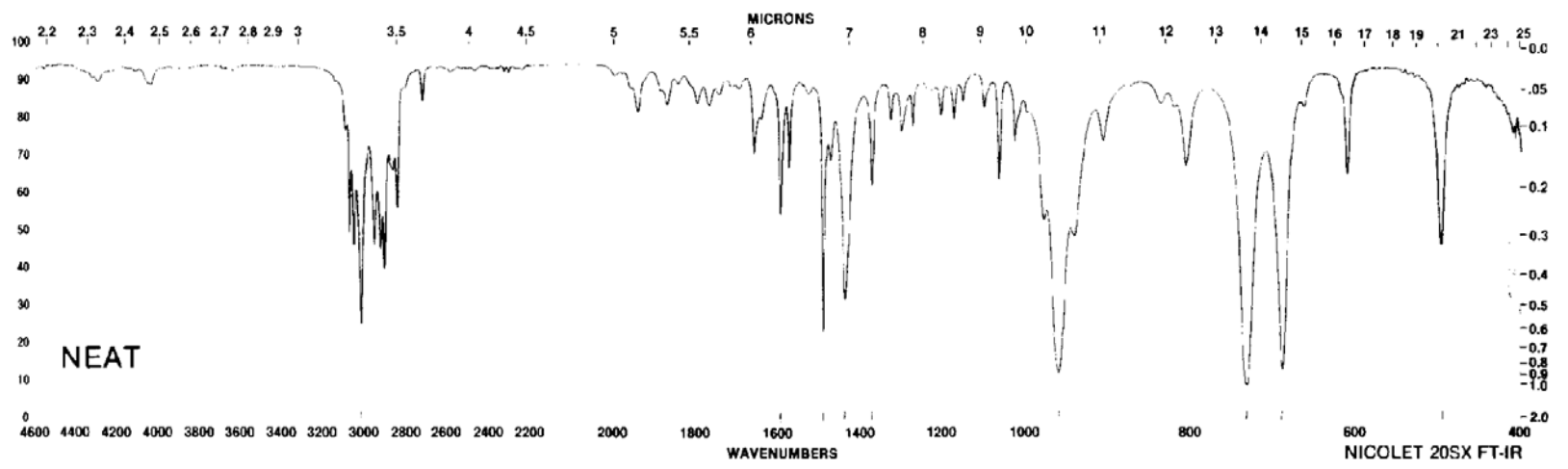
Spectral problem 5: MS interpretation

- **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)

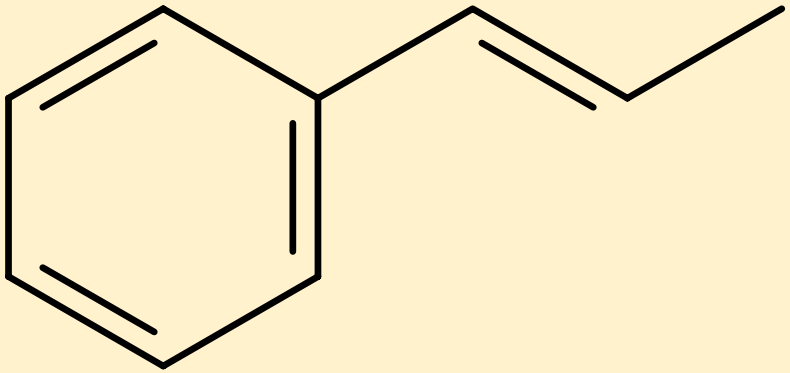
Spectral problem 5: IR/NMR



^{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