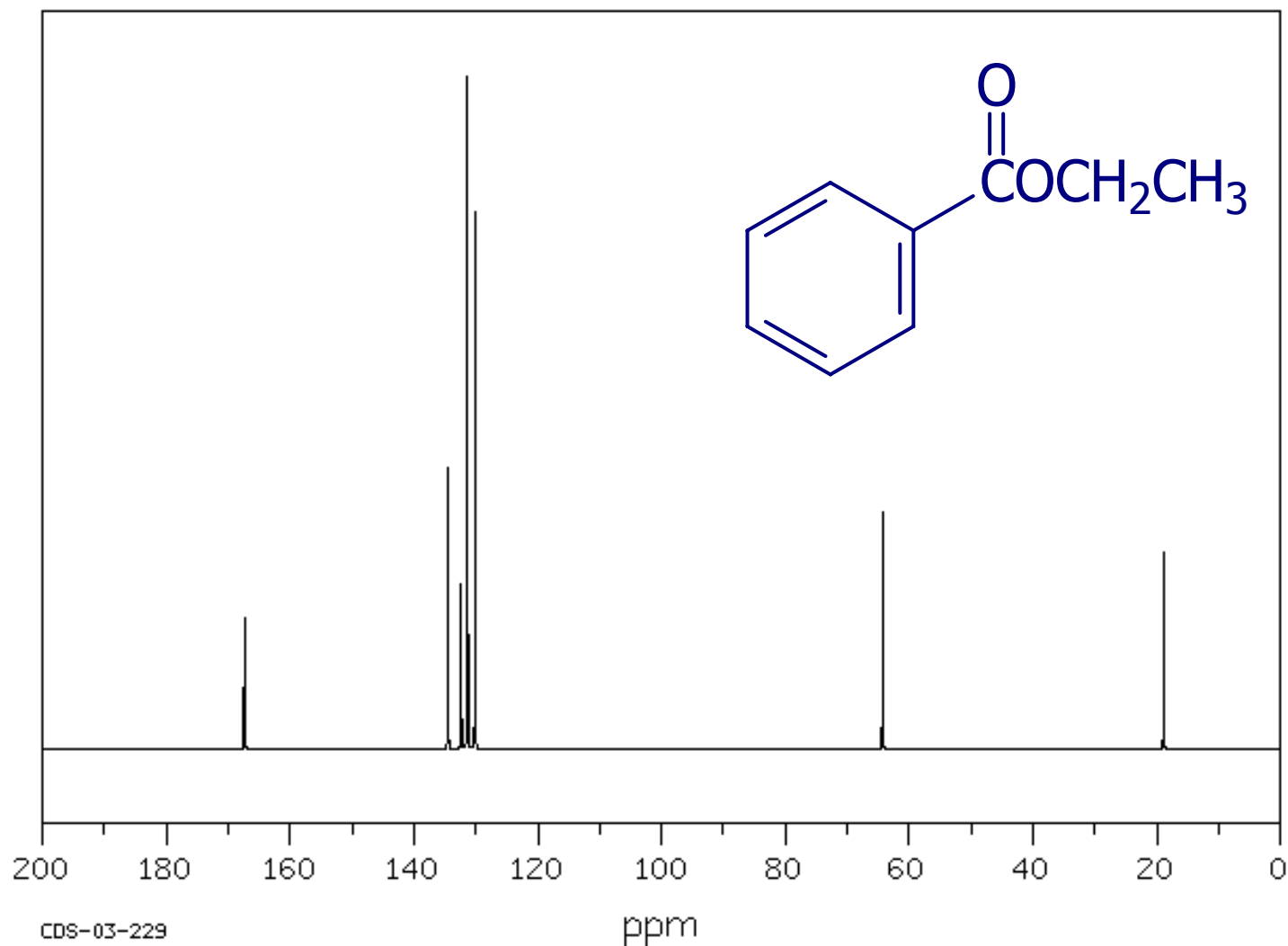


# $^{13}\text{C}$ NMR and structure determination

examples of spectroscopy problems

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



# Propose a structure

◆  $M^+ = 86$

◆ IR at  $3400\text{ cm}^{-1}$

◆  $^{13}\text{C}$  NMR:  $\delta$  30.2, 31.9, 61.8, 114.7, 138.4

◆ DEPT-90:  $\delta$  138.4

◆ DEPT-135

- Positive peak  $\delta$  138.4

- Negative peaks  $\delta$  30.2, 31.9, 61.8, 114.7

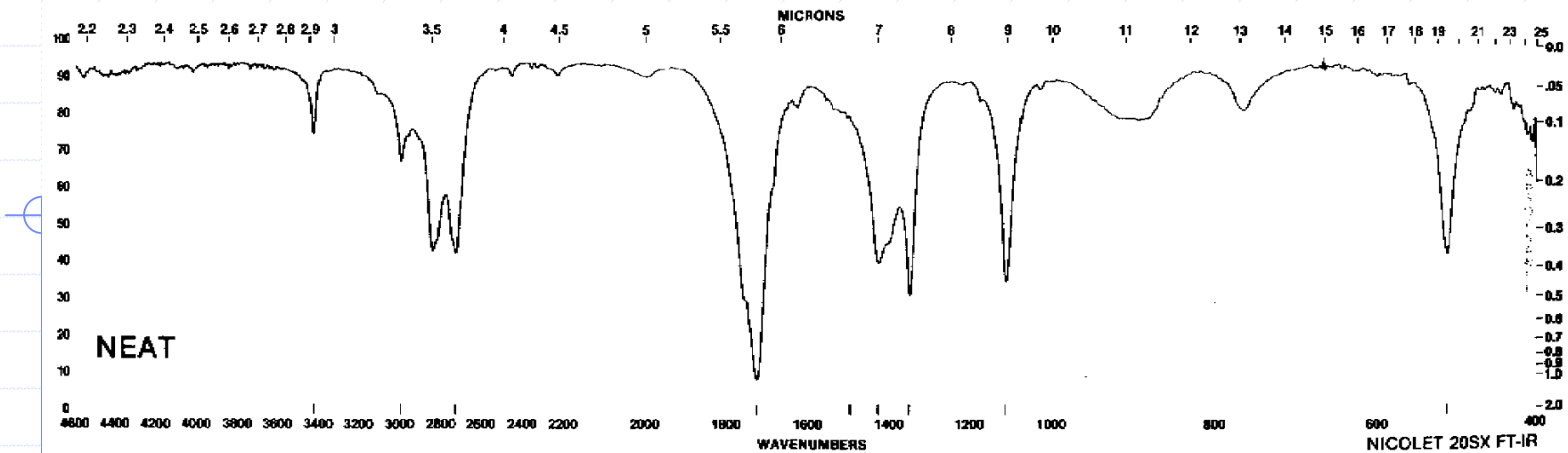
# Propose a structure

- ◆ Isomeric with previous compound
- ◆  $^{13}\text{C}$  NMR:  $\delta$  9.7, 29.9, 74.4, 114.4, 141.4
- ◆ 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

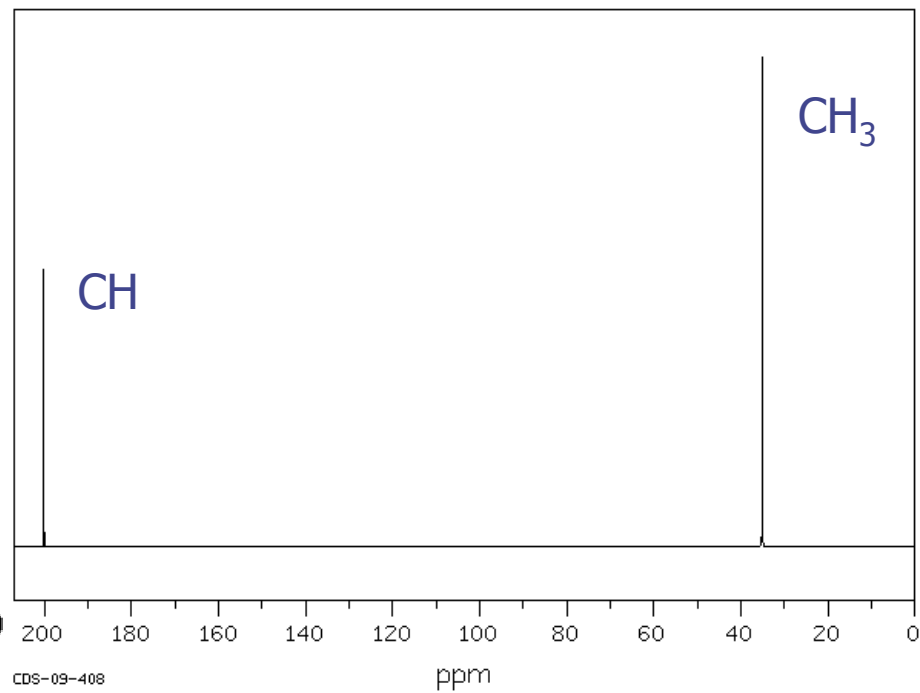
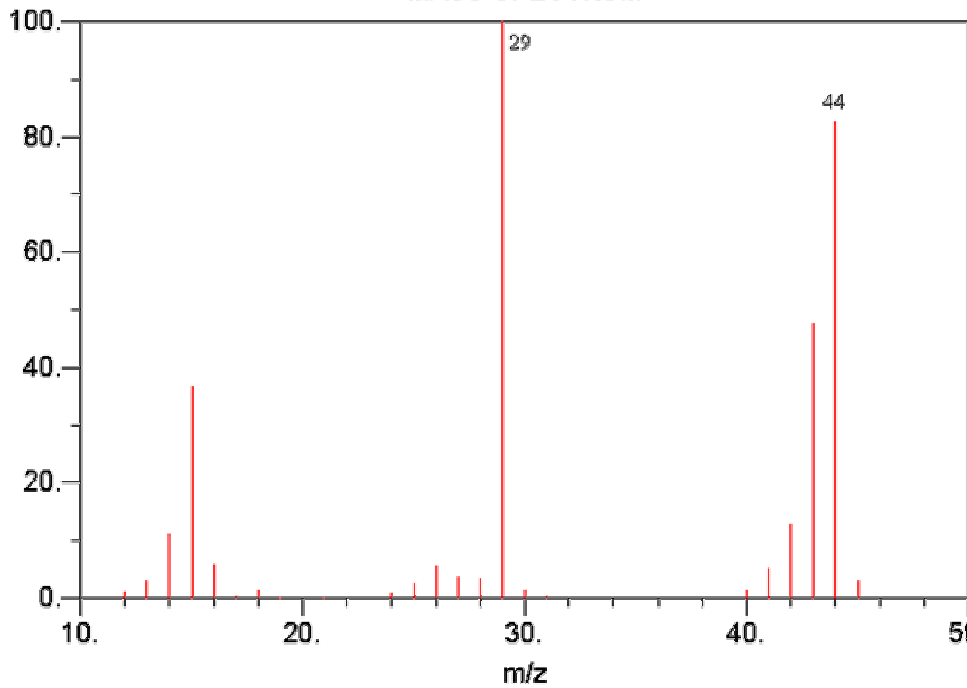
# Problem 1

◆ MW = 44

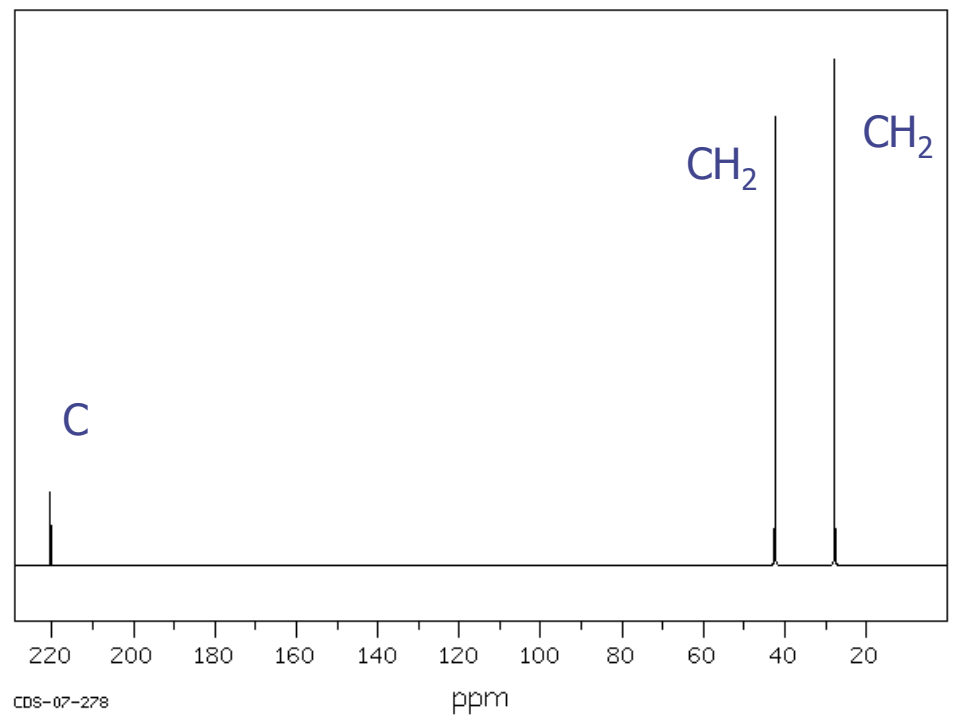
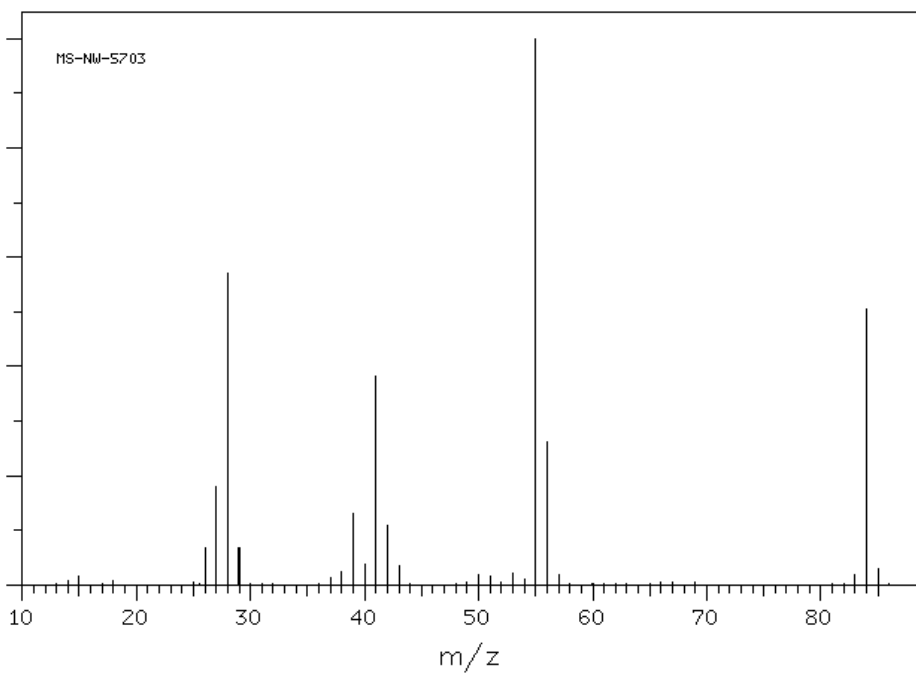
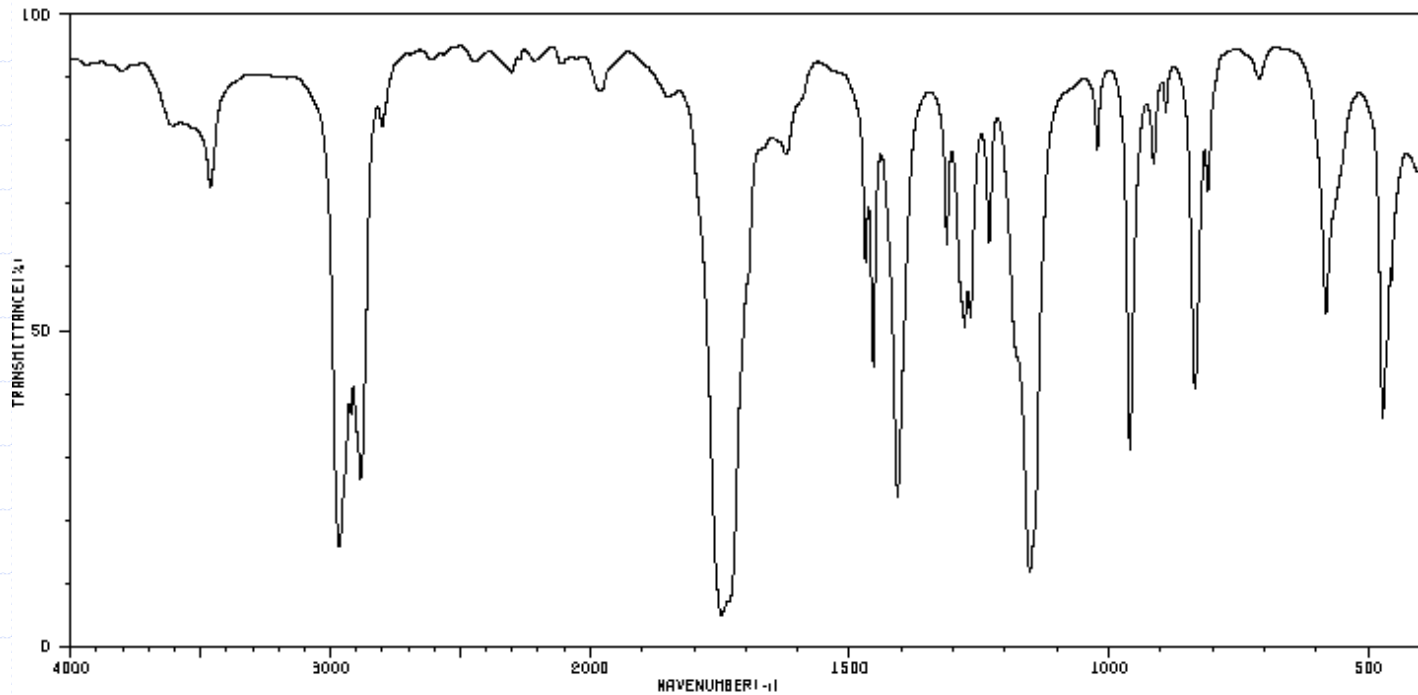
◆ Spectra on next page



MASS SPECTRUM



# Problem 2

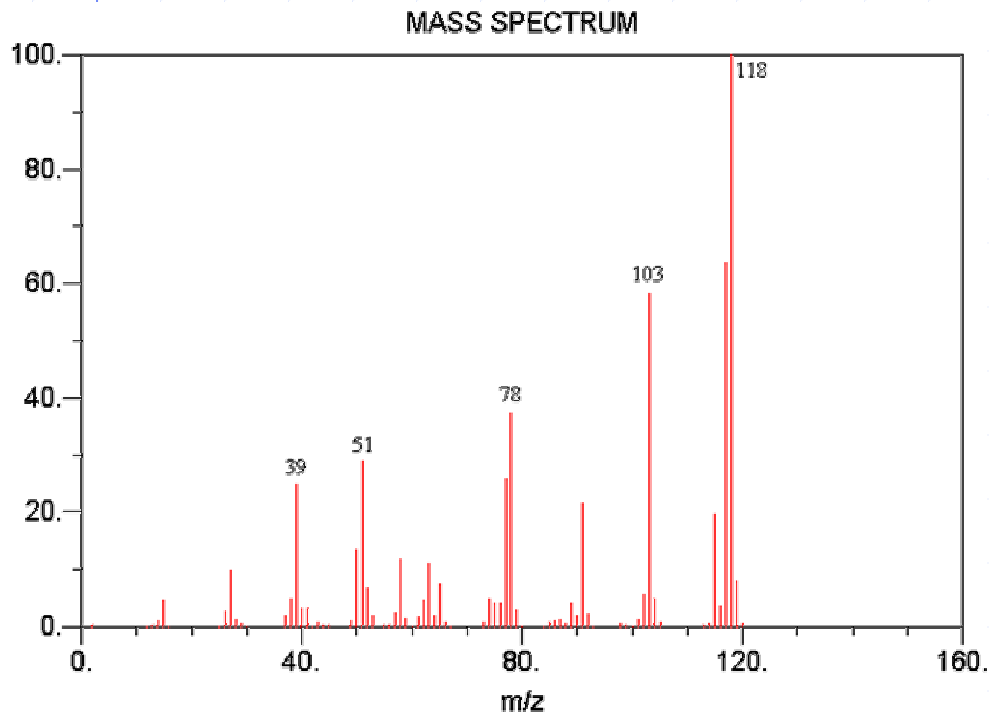
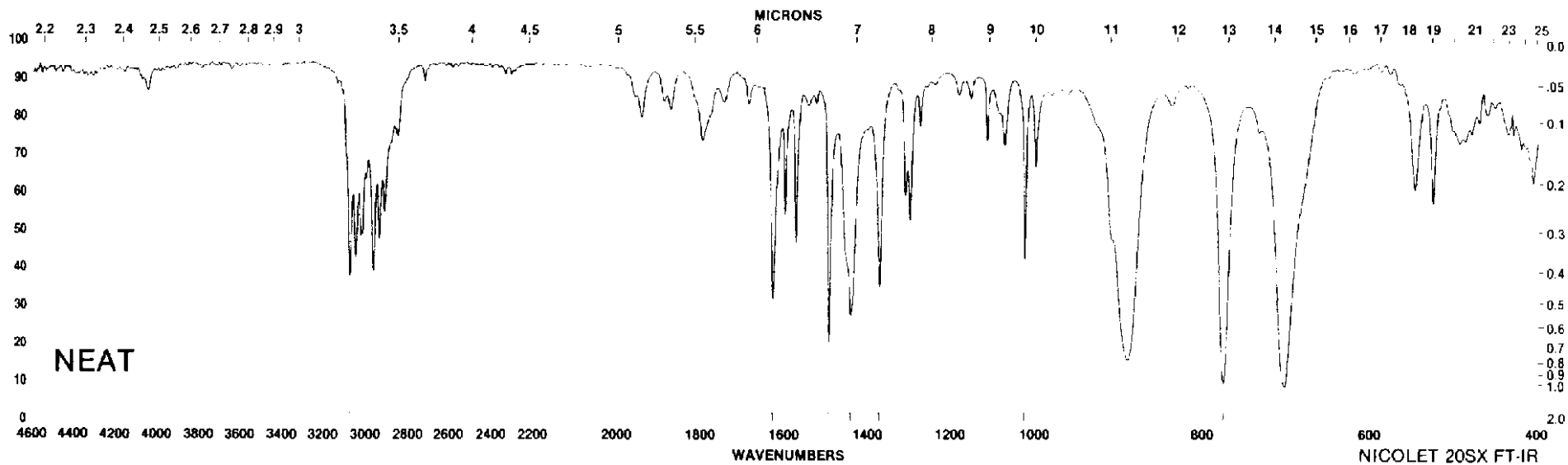


# Problem 3

◆ MW = 118

◆ Spectra on next page





$^{13}\text{C}$  NMR: 145.2(C),  
137.4(C), 128.4(CH),  
127.7(CH), 126.2(CH),  
104.9(CH<sub>2</sub>), 25.4(CH<sub>3</sub>)

# Problem 4

◆ MW = 148

◆ Spectra on next page

