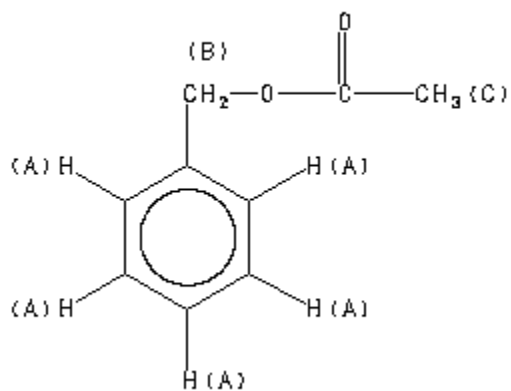


## Organic Chemistry II (CHEM 242-002)

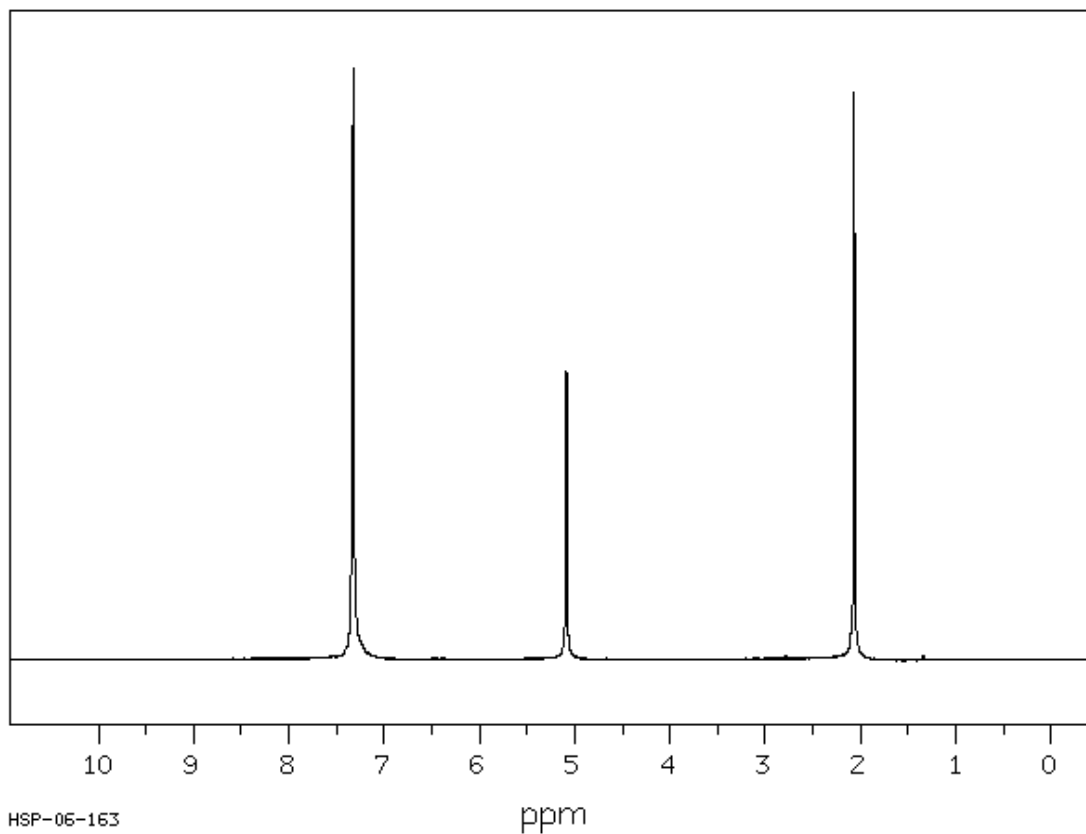
Instructor: Dr. Chulsung Bae

### Examples of $^1\text{H}$ NMR Spectra (for Chapter 13)

#### Benzyl acetate

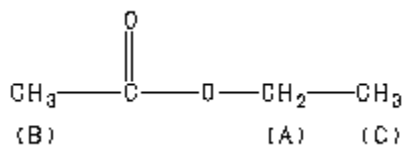


Proton	Chemical Shift in ppm
A	7.33 (5H from aromatic protons)
B	5.085 (2H, singlet)
C	2.064 (3H, singlet)

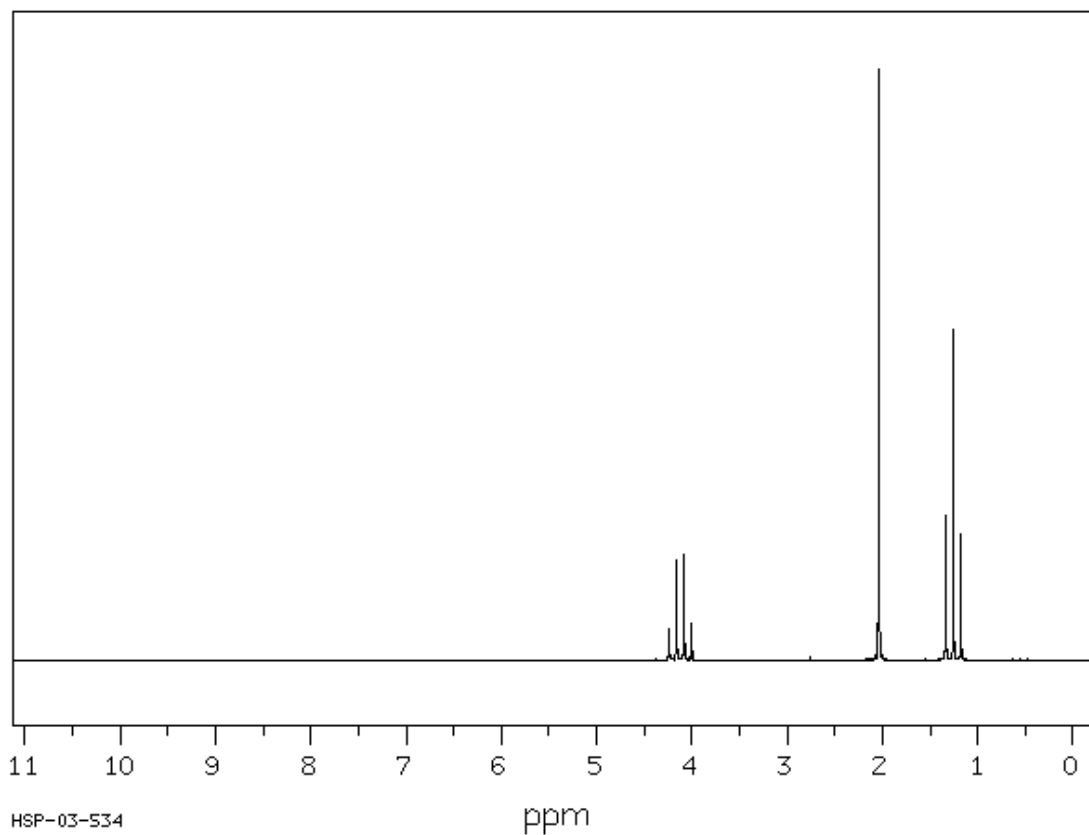


HSP-06-163

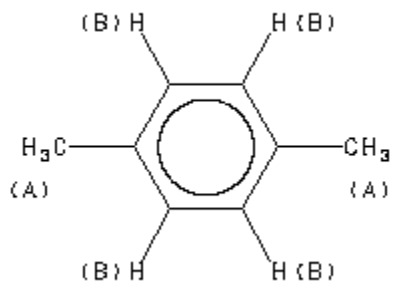
## Ethyl acetate



Proton	Chemical Shift in ppm
A	4.119 (2H, quartet, $J_{A-C} = 7.1$ HZ)
B	2.038 (3H, singlet)
C	1.260 (3H, triplet, $J_{A-C} = 7.1$ HZ)



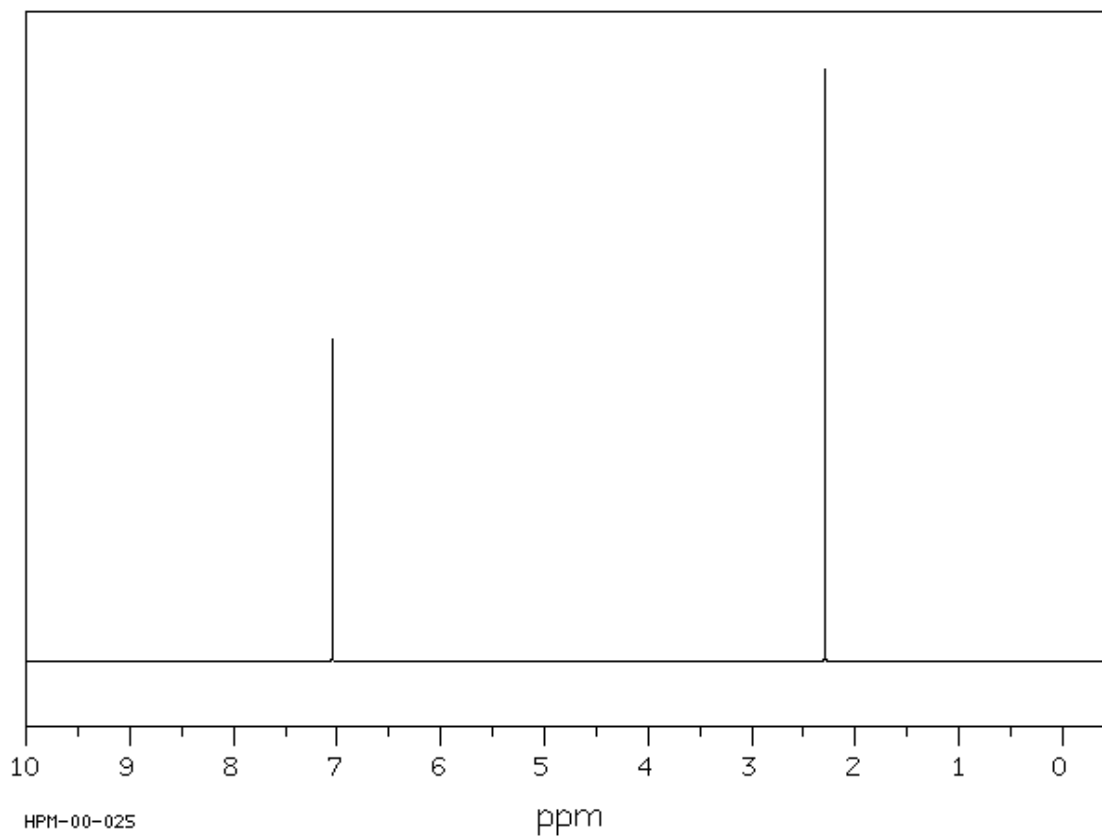
## p-Xylene



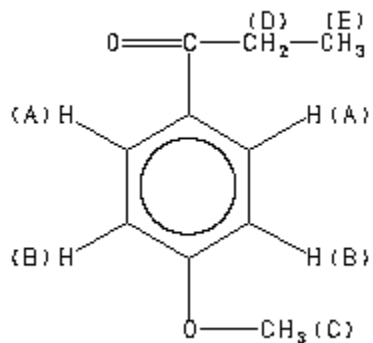
### Proton    Chemical shift in ppm

A    2.296 (6H, singlet)

B    7.046 (4H, singlet)

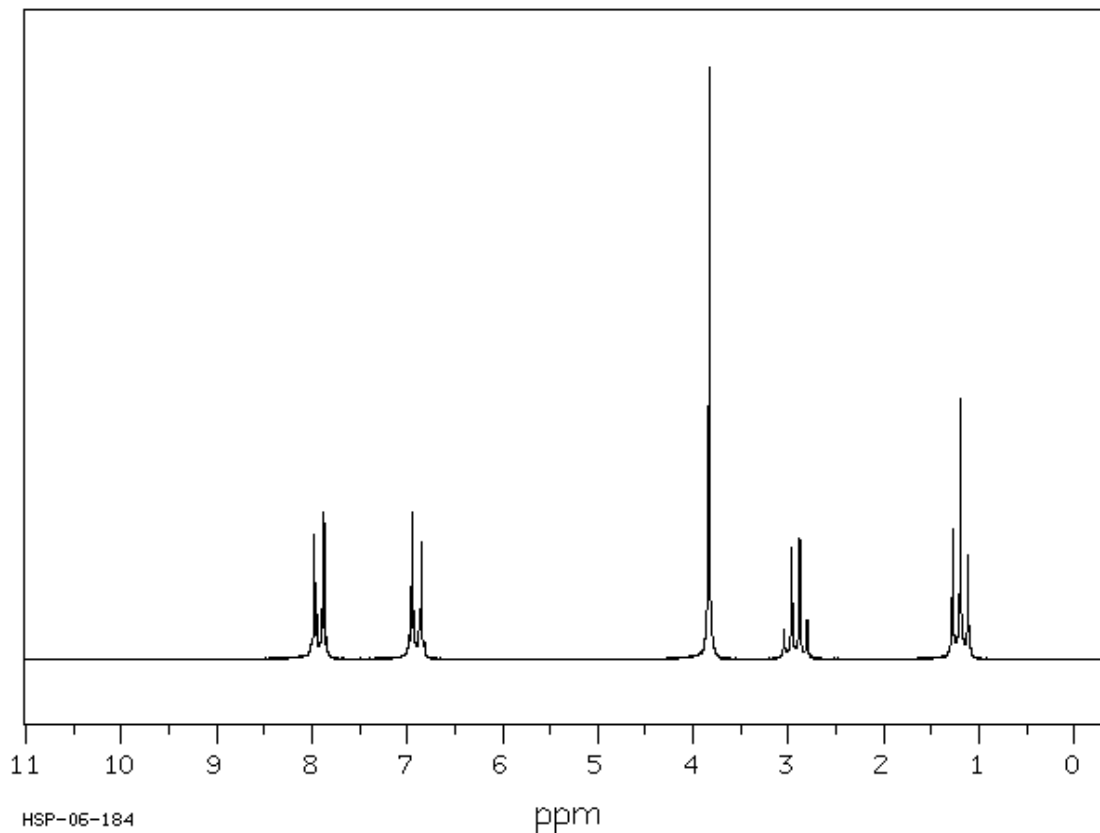


## p-Methoxypropiofenone

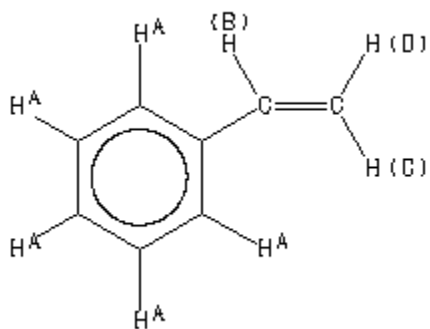


### Proton      Chemical Shift in ppm

A	7.922 (2H, doublet due to coupling with H <sub>B</sub> , J <sub>A-B</sub> = 9.1 Hz)
B	6.907 (2H, doublet due to coupling with H <sub>A</sub> , J <sub>A-B</sub> = 9.1 Hz)
C	3.830 (3H, singlet)
D	2.918 (2H, quartet due to coupling with CH <sub>3</sub> , J <sub>D-E</sub> = 7.2 Hz)
E	1.198 (3H, triplet due to coupling with CH <sub>2</sub> , J <sub>D-E</sub> = 7.2 Hz)

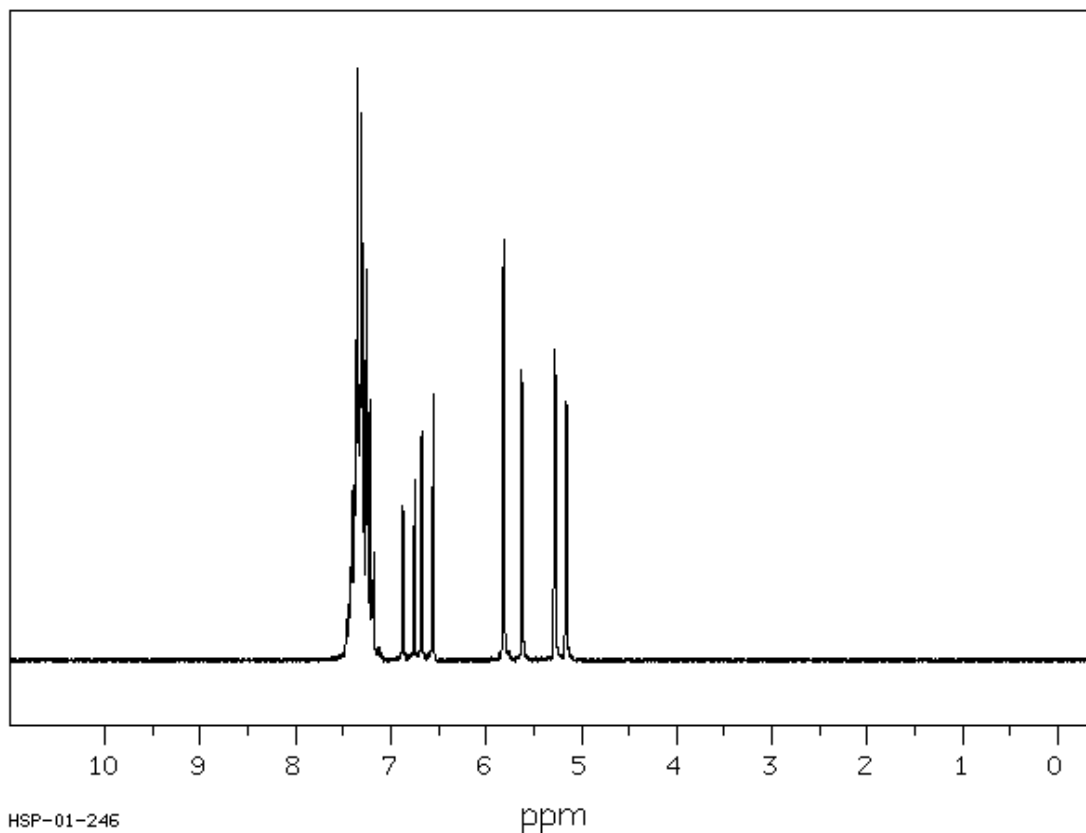


## Styrene

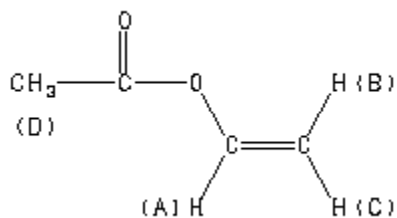


Proton	Chemical Shift in ppm
A	7.50 to 7.10 (5H from aromatic ring)
B	6.692 (1H, doublet of doublet, $J_{B-C} = 17.6$ Hz, $J_{B-D} = 10.8$ Hz)
C	5.737 (1H, doublet, $J_{B-C} = 17.6$ Hz),
D	5.225 (1H, doublet, $J_{B-D} = 10.8$ Hz)

Coupling constant due to protons at trans position ( $J_{B-C}$ ) is always larger than that of cis position ( $J_{B-D}$ ).



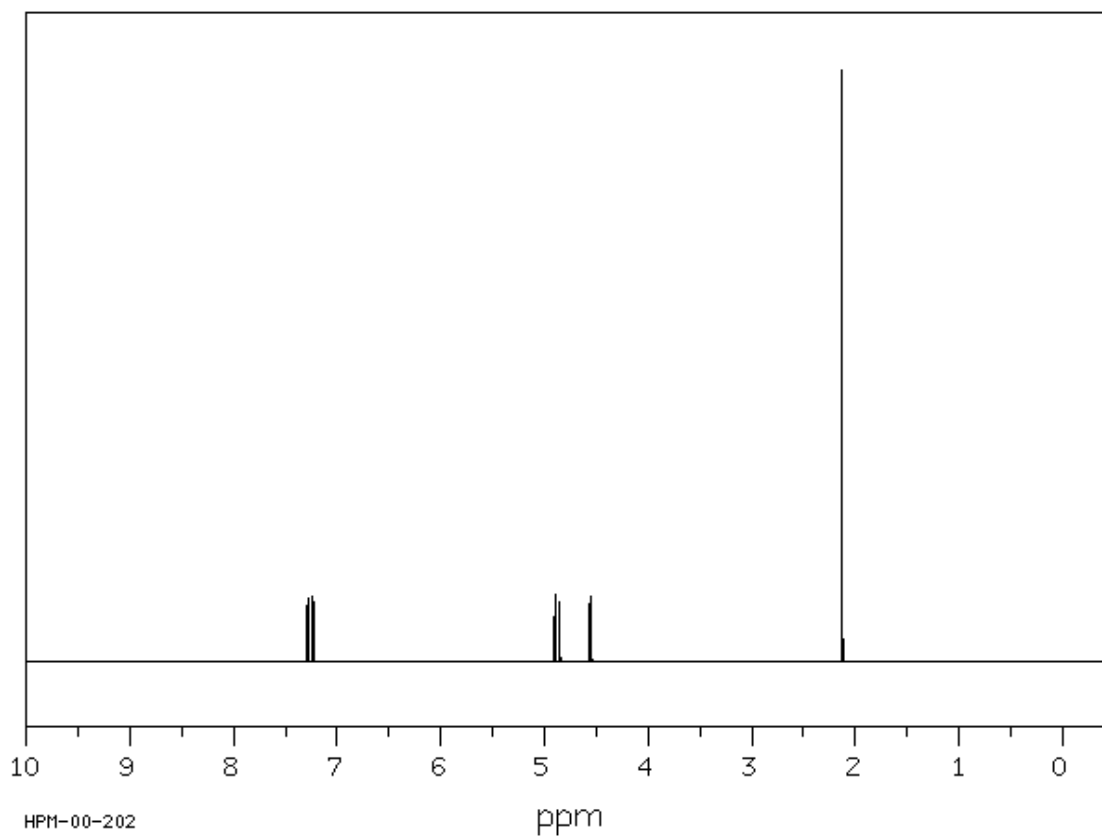
## Vinyl acetate



### Proton ppm

- A 7.260 (1H, doublet of doublet,  $J_{A-B} = 13.98$  Hz,  $J_{A-C} = 6.31$  Hz)
- B 4.879 (1H, doublet,  $J_{A-B} = 13.98$  Hz)
- C 4.563 (1H, doublet,  $J_{A-C} = 6.31$  Hz)
- D 2.131 (3H, singlet)

Coupling constant due to protons at trans position ( $J_{A-B}$ ) is always larger than that of cis position ( $J_{A-C}$ ).

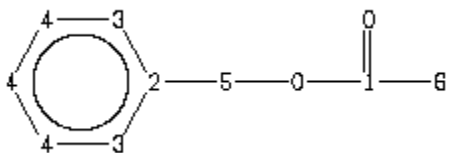


# Organic Chemistry II (CHEM 242-002)

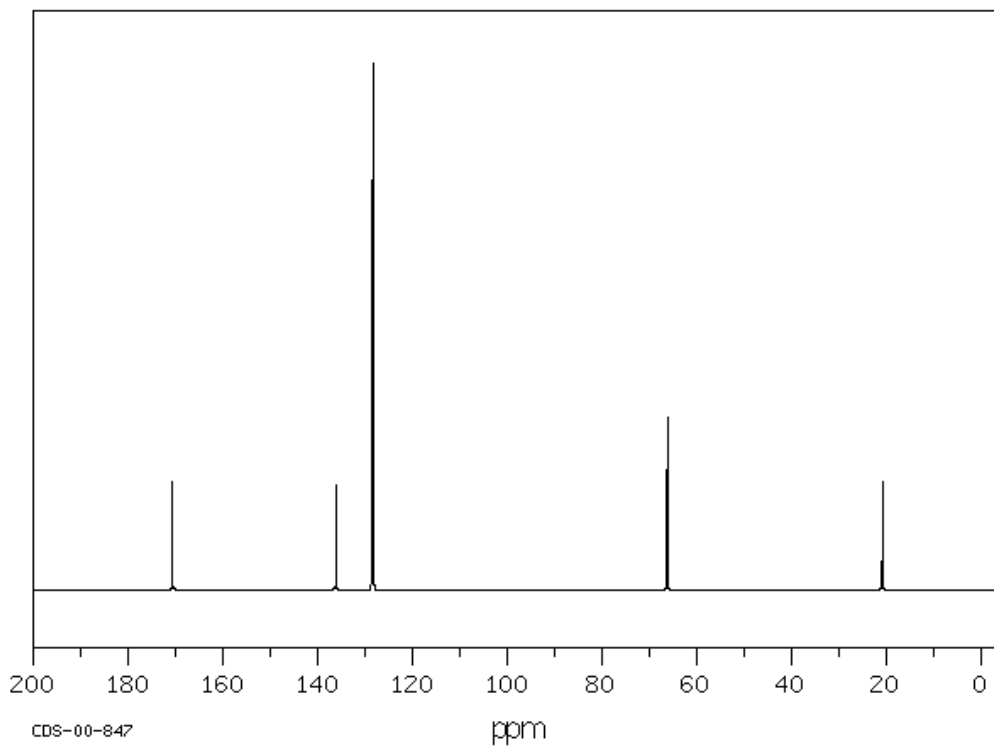
Instructor: Dr. Chulsung Bae

## Examples of $^{13}\text{C}$ NMR Spectra (for Chapter 13)

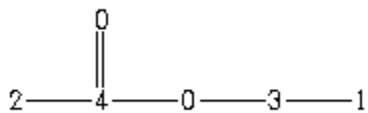
Benzyl acetate



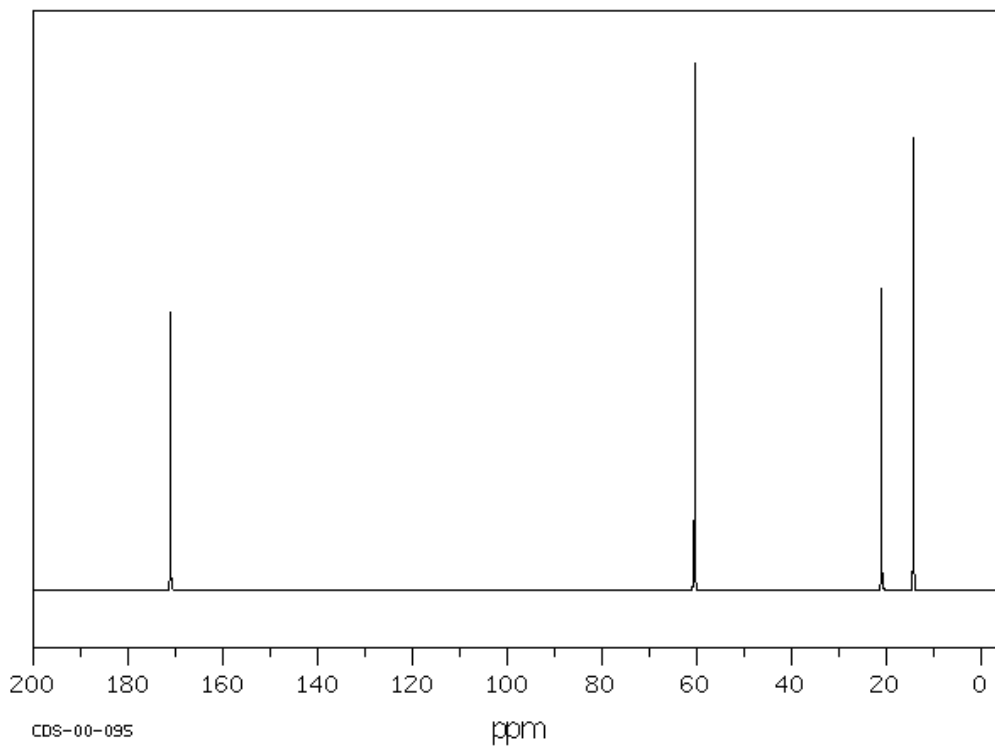
ppm	Int.	Assign.
170.70	204	C1
136.14	199	C2
128.56	776	C3
128.24	1000	C4
66.24	328	C5
20.82	204	C6



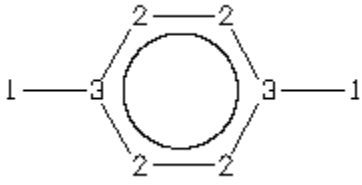
## Ethyl acetate



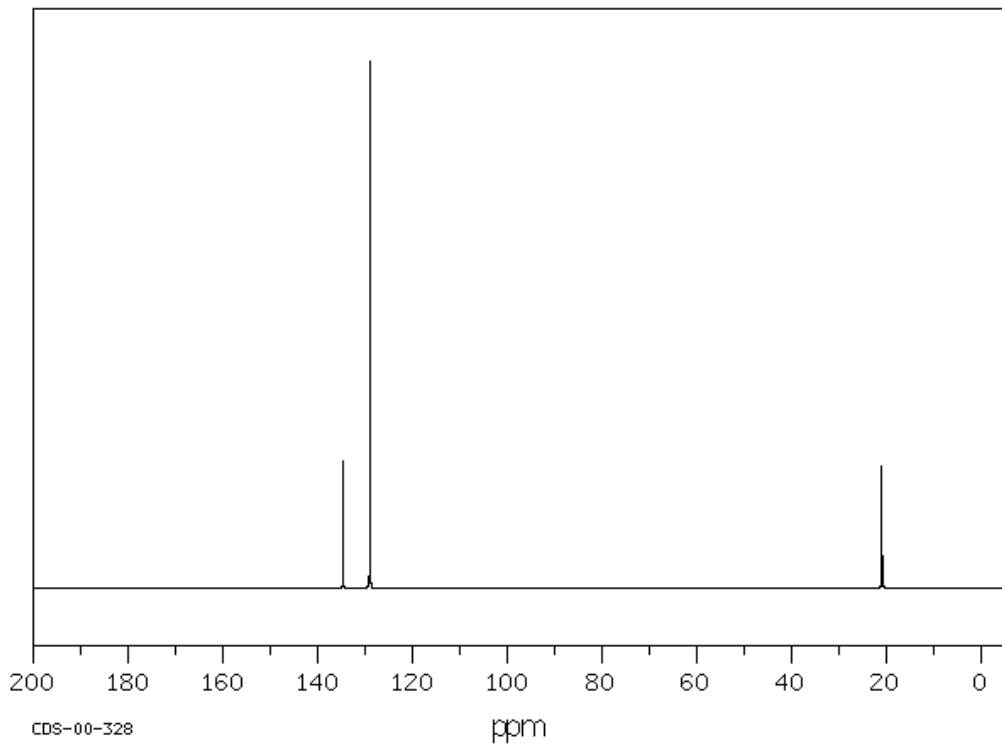
ppm	Int.	Assign.
171.08	527	C4
60.44	1000	C3
21.00	571	C2
14.28	857	C1



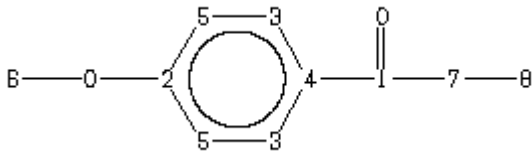
# p-Xylene



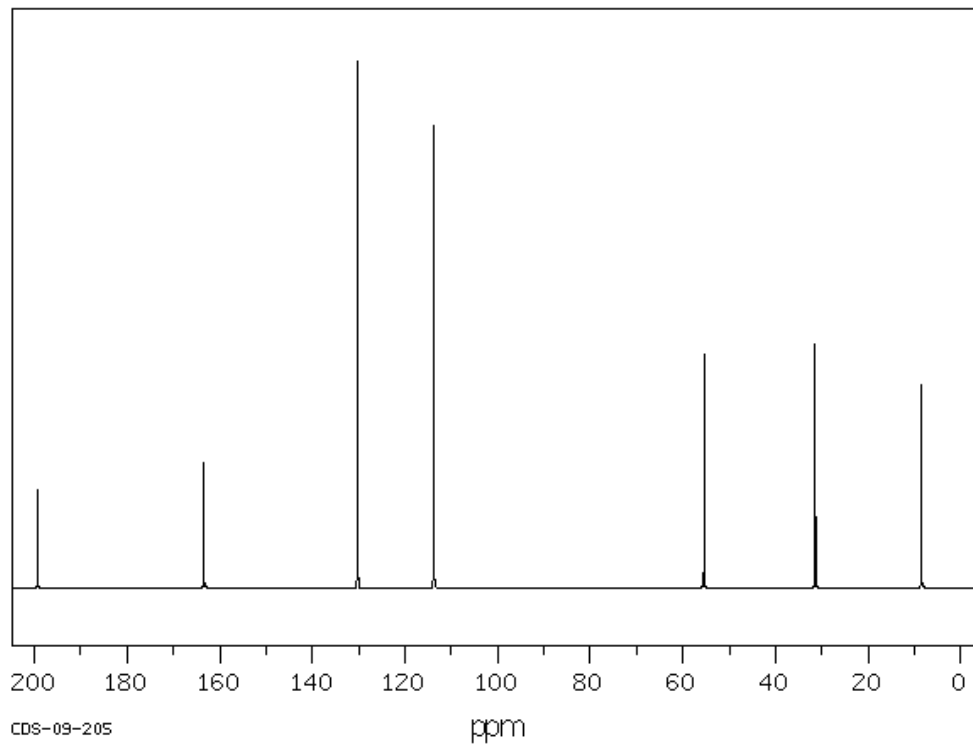
ppm	Int.	Assign.
134.66	239	3
128.97	1000	2
20.90	229	1



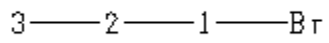
## p-Methoxypropiophenone



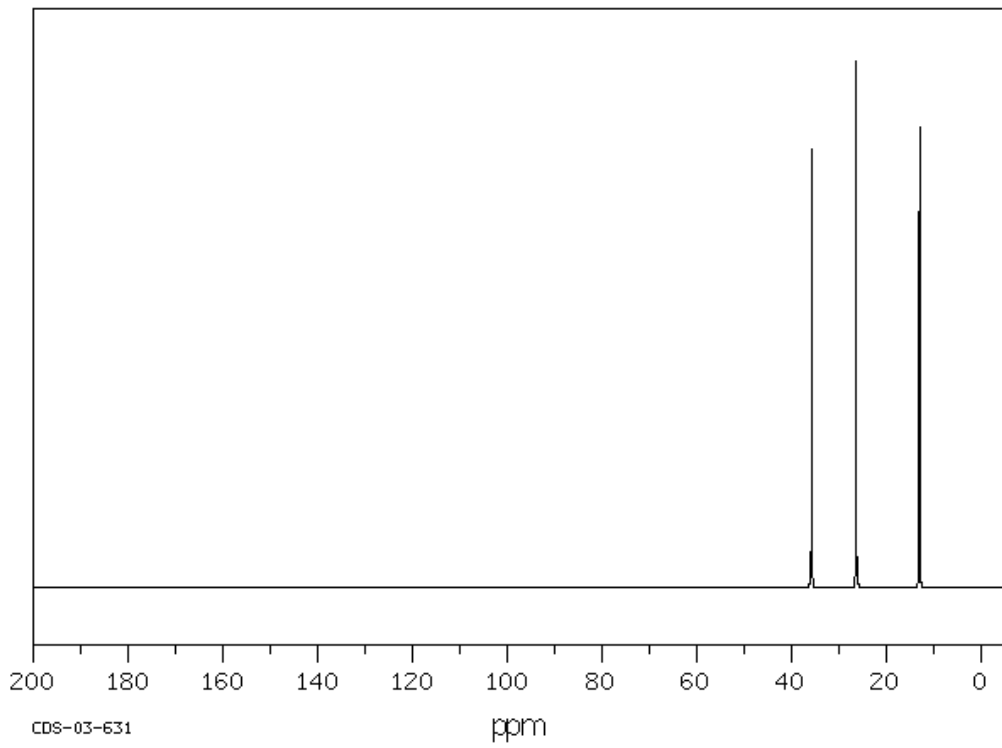
ppm	Int.	Assign.
199.30	185	C1
163.39	237	C2
130.21	1000	C3
Not detected (too small)		C4
113.74	876	C5
55.39	441	C6
31.39	463	C7
8.45	386	C8



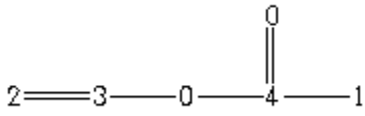
# 1-Bromopropane



ppm	Int.	Assign.
35.76	833	C1
26.36	1000	C2
12.99	873	C3



# Vinyl acetate



ppm	Int.	Assign.
167.95	505	C4
141.38	1000	C3
97.54	880	C2
20.61	462	C1

