

4.18: Solutions to Selected Problems

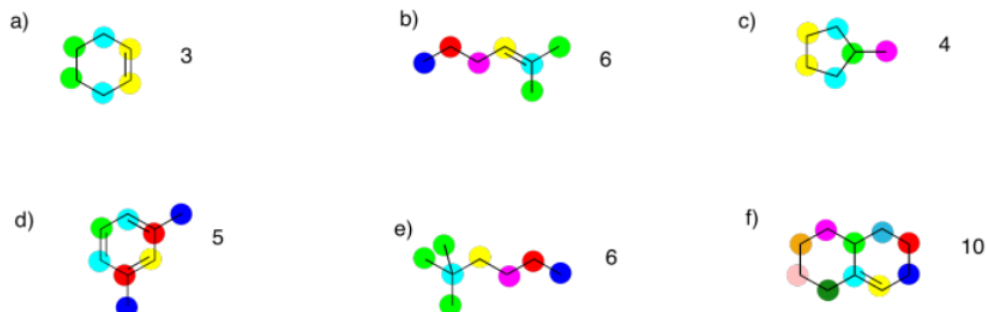
Exercise 4.2.1:

a) 10 ppm b) 64 ppm c) 158 ppm

Exercise 4.2.2:

a) 63 ppm b) 201 ppm c) 71 ppm

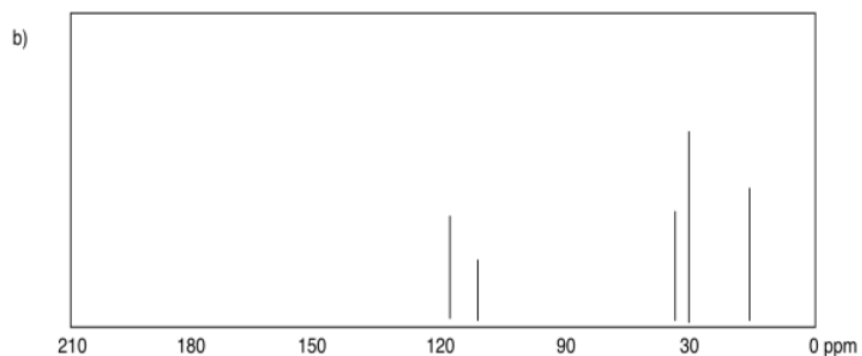
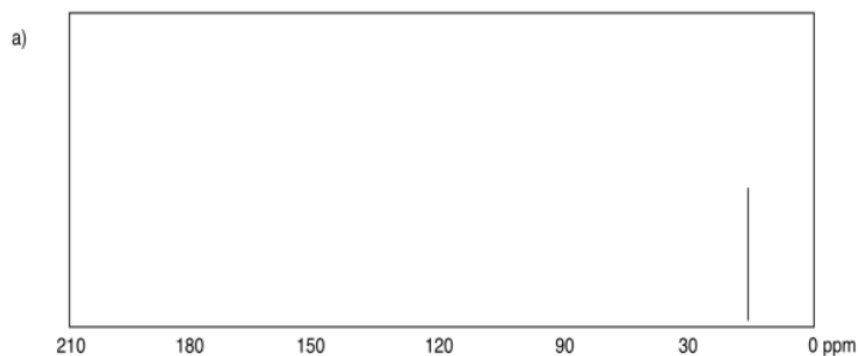
Exercise 4.3.1:

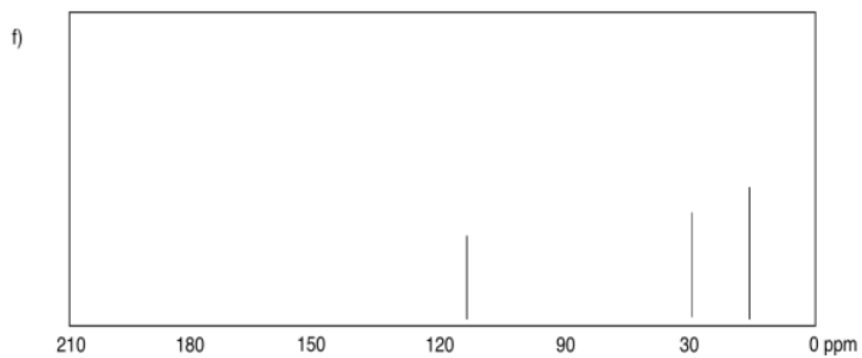
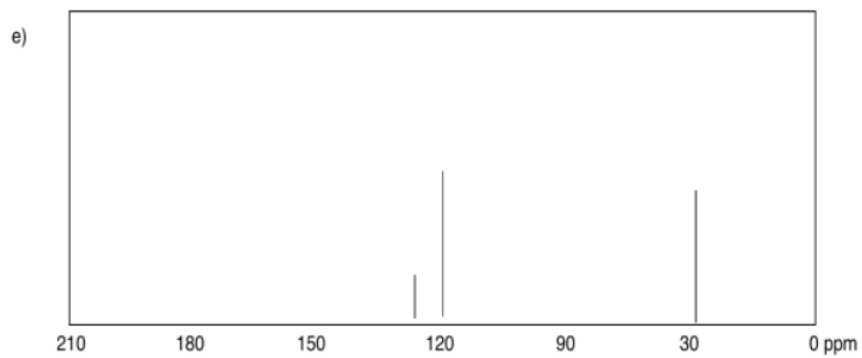
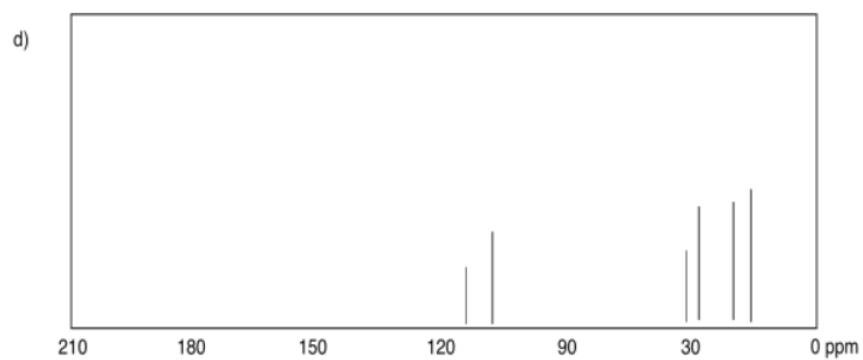
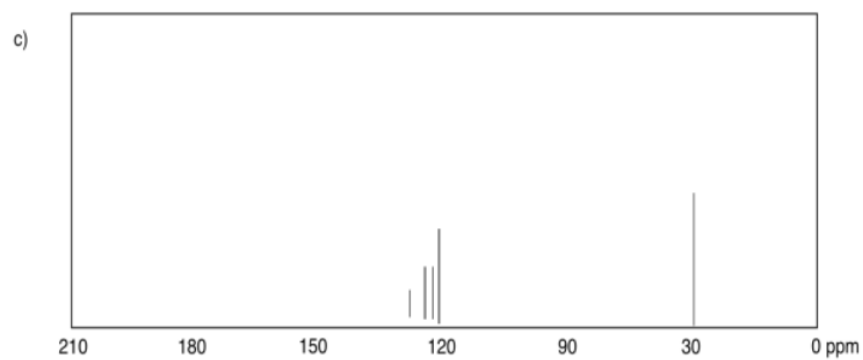


Exercise 4.3.2:

- pentane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$, or hexane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$
- heptane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$, or octane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$
- nonane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$, or decane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$

Exercise 4.4.1:

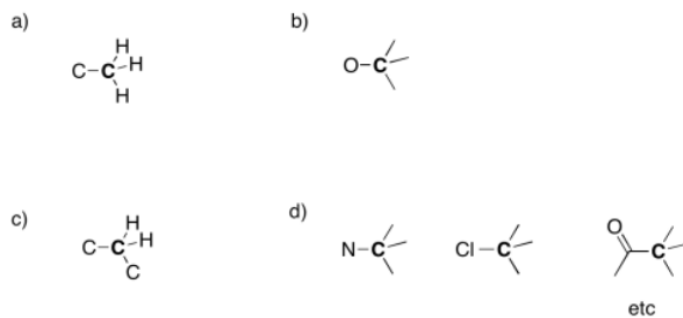




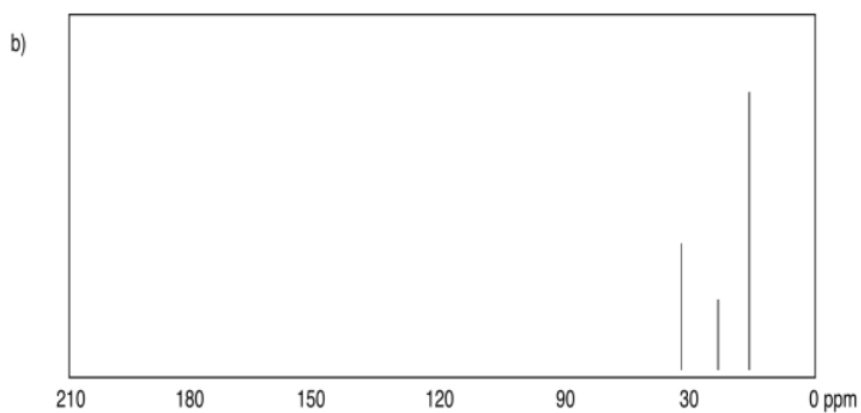
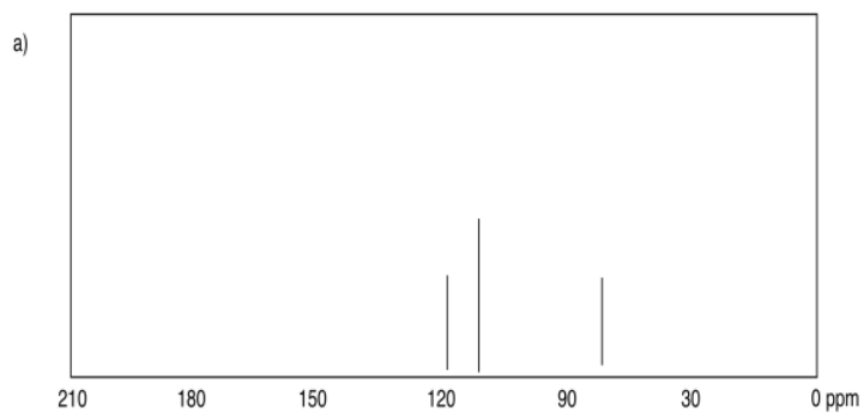
Exercise 4.4.2:

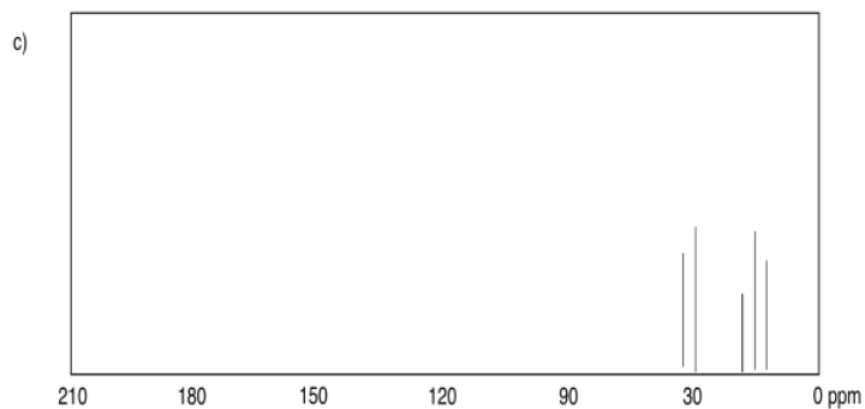
a) sp^3 b) sp^2 c) sp^2 d) sp^3 e) sp^3 f) sp^2

Exercise 4.5.1:



Exercise 4.5.2:



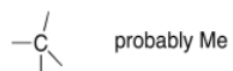


Exercise 4.6.1:

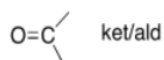
a) 127 ppm



b) 11 ppm



c) 196 ppm



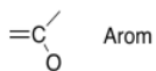
d) 65 ppm



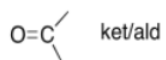
e) 111 ppm



f) 154 ppm



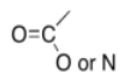
g) 210 ppm



h) 28 ppm



i) 170 ppm

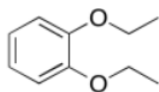


j) 42 ppm

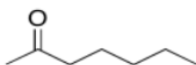


Exercise 4.6.2:

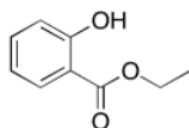
a)



b)



c)



Exercise 4.8.1:

a) H-C_{sp}3 b) H-C_{sp}3 c) H-C_{sp}2 d) H-C_{sp}3 e) H-C_{sp}2 f) H-C_{sp}2 g) H-C_{sp}3

Exercise 4.8.2:

a) carbon b) carbon c) nitrogen d) oxygen e) carbon f) oxygen g) nitrogen

Exercise 4.8.3:

a) aromatic b) aromatic c) alkene d) alkene e) alkene f) aromatic

Exercise 4.8.4:

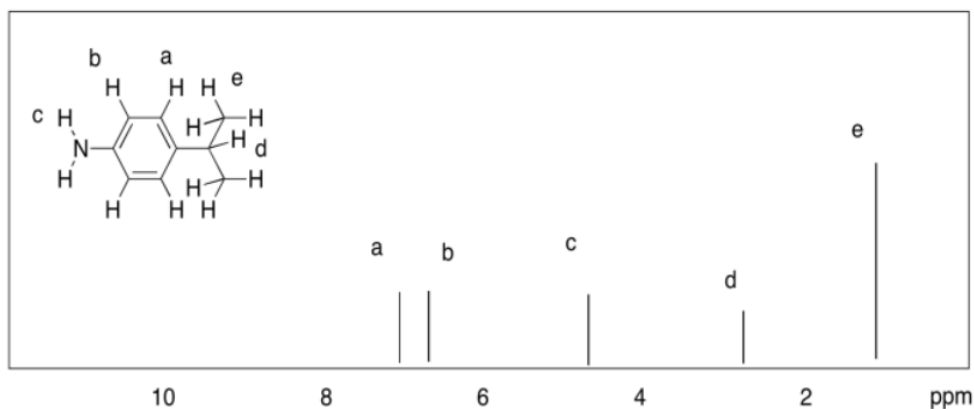
a) H-C_{Ar}-C b) H-C_{Ar}-C c) H-C_{Ar}-N d) C=O e) C=O f) H-C_{Ar}-N g) H-C_{Ar}-N

Exercise 4.8.5:

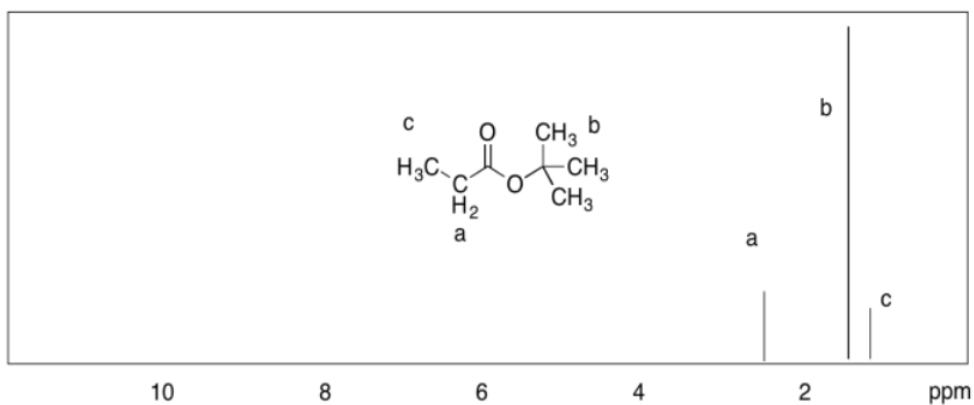
- a. 3.4 ppm: H_a 1.5 ppm: H_b, H_c 0.9 ppm: H_d
- b. 7.4 ppm: H_d 6.9 ppm: H_b, H_c 3.7 ppm: H_a
- c. 10.1 ppm: H_a 7.9 ppm: H_b 7.6 ppm: H_d 7.5 ppm: H_c
- d. 7.9 ppm: H_b 7.6 ppm: H_d 7.4 ppm: H_c 2.5 ppm: H_a

Exercise 4.8.6:

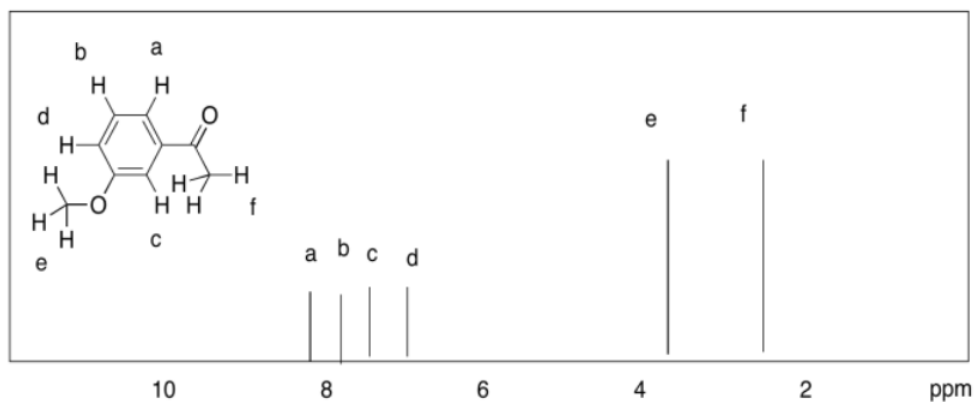
a)



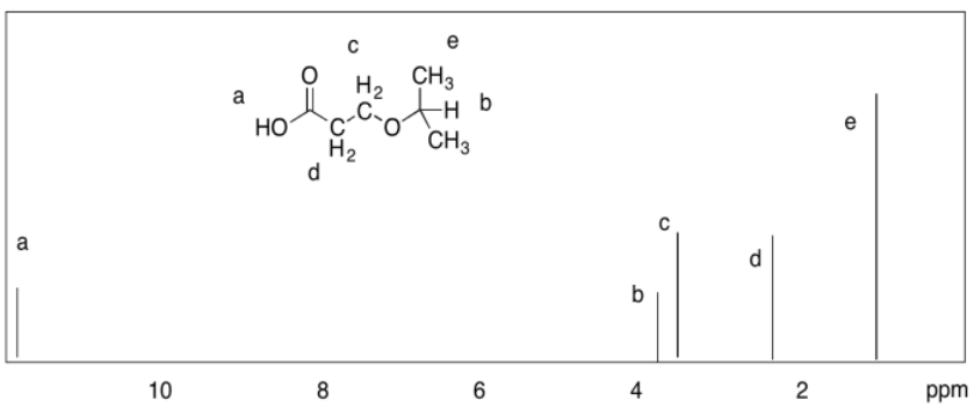
b)



c)



d)

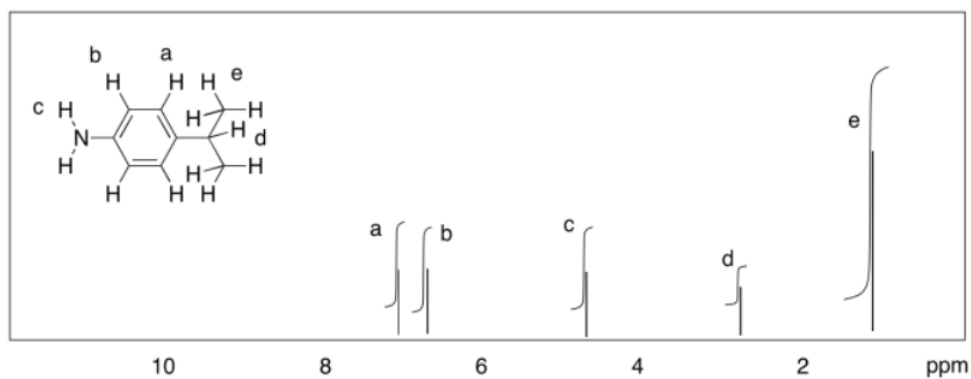


Exercise 4.9.1:

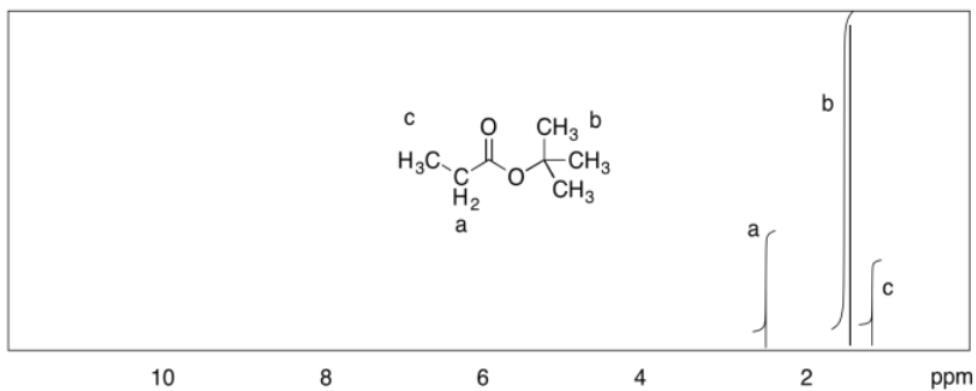
- a. 0.9 ppm, 6H; 1.0 ppm, 6H (1:1 ratio)
- b. 0.9 ppm, 6H; 1.0 ppm, 12H (1:2 ratio)
- c. 0.9 ppm, 6H; 1.0 ppm, 16H (3:8 ratio)
- d. 0.9 ppm, 6H; 1.0 ppm, 10H (3:5 ratio)
- e. 0.9 ppm, 6H; 1.0 ppm, 8H (3:4 ratio)

Exercise 4.9.2:

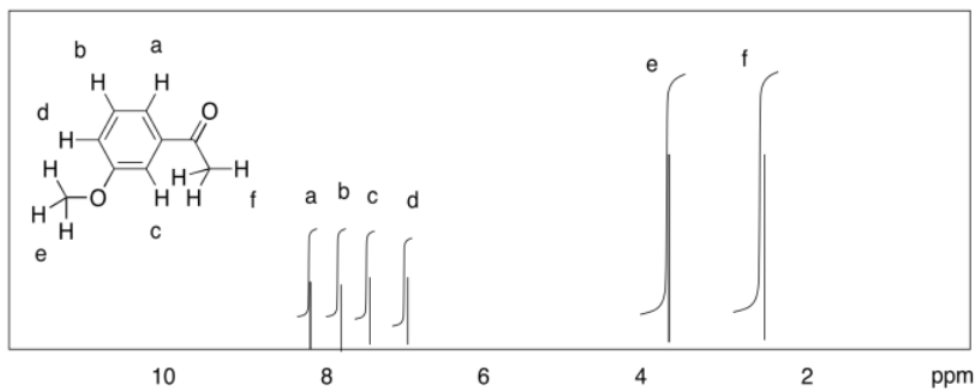
a)



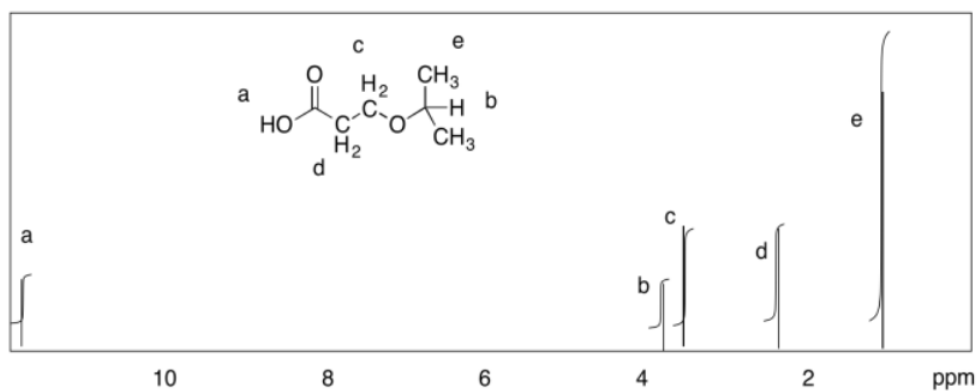
b)



c)



d)



Exercise 4.9.3:

a) 5:2:3

Exercise 4.10.1:

(There will be some variation in the shift depending on the rest of the structure; this is just an estimate.)

a) 3.5 ppm, quartet, 2H b) 1.5 ppm, sextet, 2H c) 2.6 ppm, septet, 1H

d) 2.3 ppm, quintet, 1H e) 2.2 ppm, quartet, 2H f) 1.7 ppm, nonet, 1H

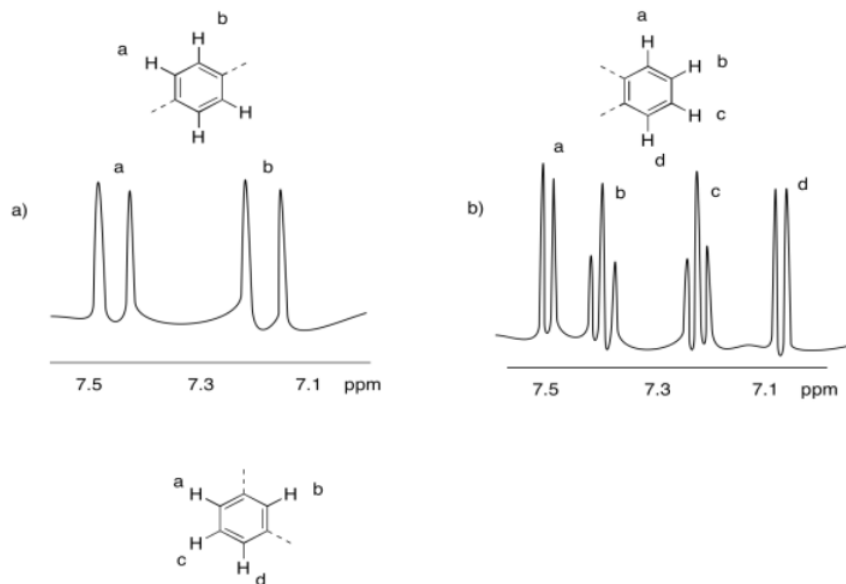
Exercise 4.10.2:

(There will be some variation in the shift depending on the rest of the structure; this is just an estimate.)

a) 7.8 ppm, doublet, 1H b) 8.4 ppm, singlet, 1H c) 6.7 ppm, singlet, 1H

d) 7.2 ppm, triplet, 1H e) 6.9 ppm, doublet, 1H

Exercise 4.10.3:



Exercise 4.10.4:

3.4 ppm, doublet: CH-CH₂-O

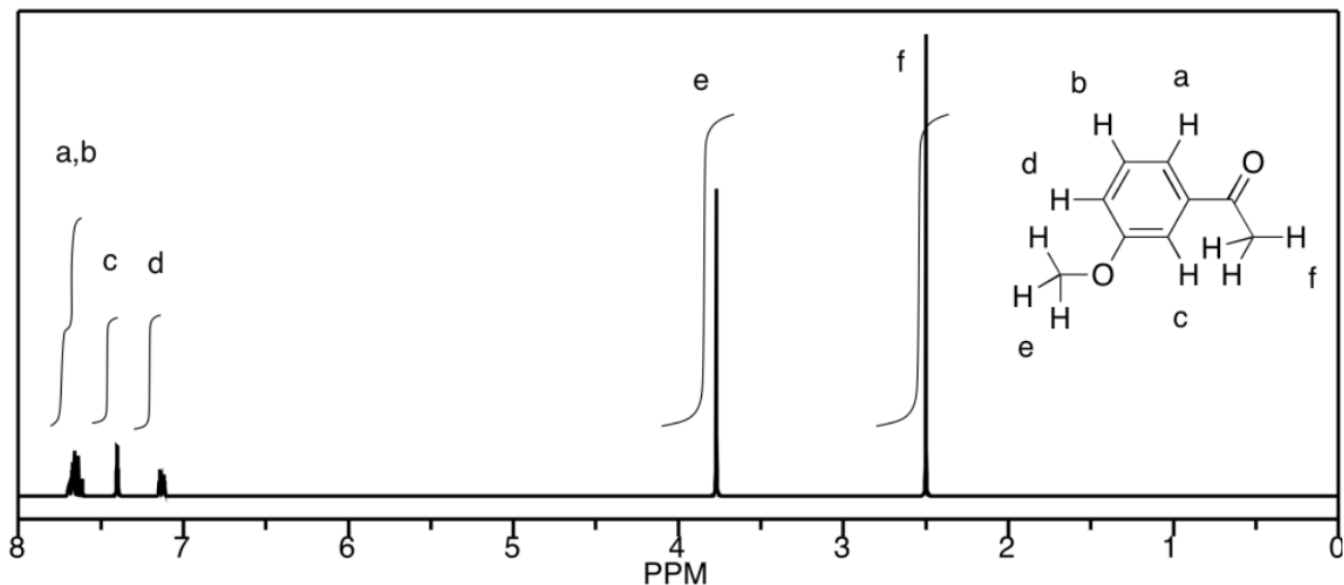
2.1 ppm, singlet: OH

1.7 ppm, nonet: (CH₃)₂CHCH₂

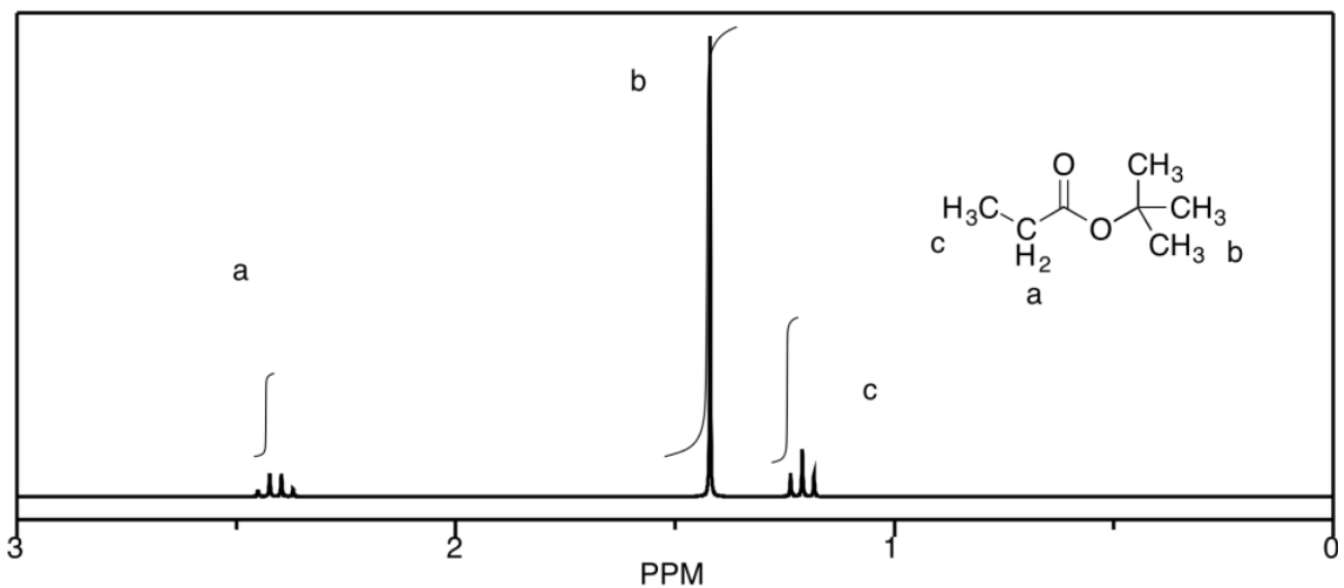
0.9 ppm, doublet: CH(CH₃)₂

Exercise 4.10.5:

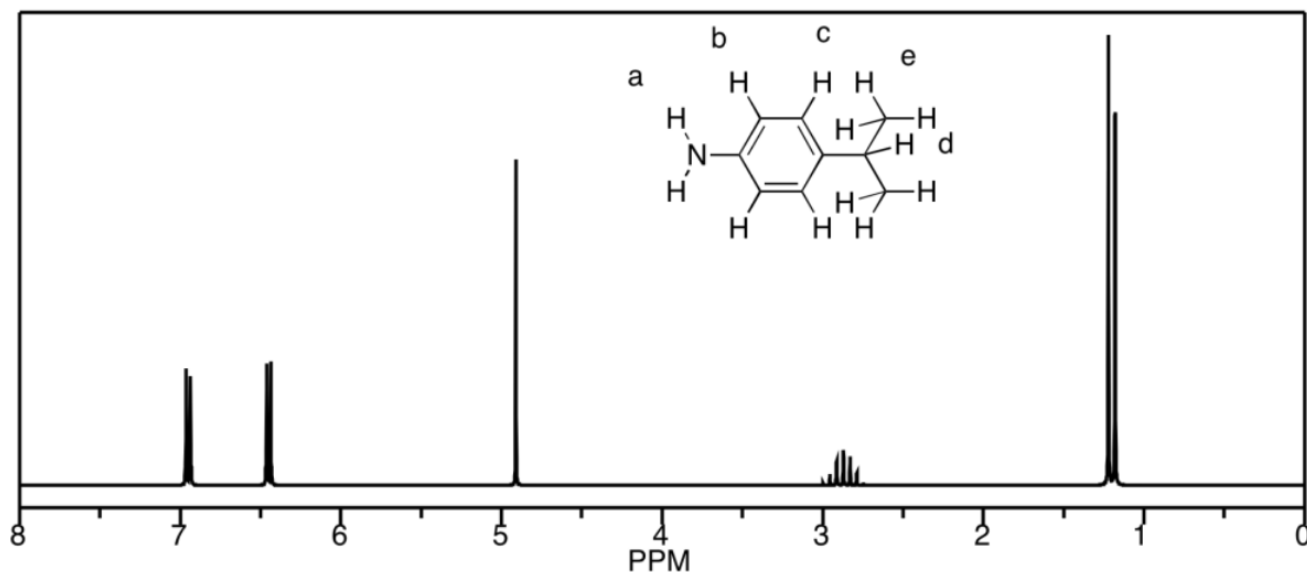
a) This is a simulated spectrum. The peaks at f, e, and c are singlets. The peak at d is a doublet. The peaks at a & b are unfortunately coincident, so their multiplicities are obscured, but they would be doublets & triplets, respectively.



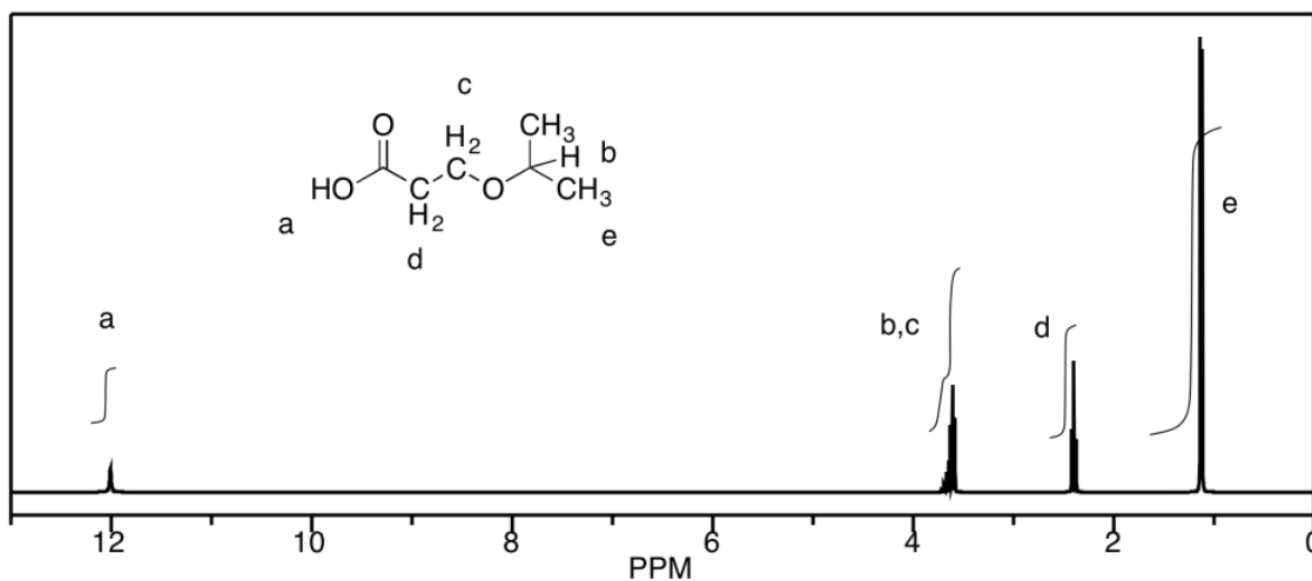
b)



c)



d) The peaks at b and c unfortunately coincide, but they would be a septet and a triplet, respectively. Otherwise, a is a singlet, d is a triplet, and e is a doublet.



Exercise 4.12.1:

Fill in partial structures for the following peaks.

Aromatic (benzene etc) peaks are labeled "Ar" to distinguish from alkene peaks that show up further upfield (lower shift). Also, some peaks may be in two symmetric positions and are labeled with "x2".

- a) 10.1 ppm, 1H, triplet, $\text{CH}_2\text{-CH=O}$ b) 3.4 ppm, 1H, septet, $\text{O-CH(CH}_3)_2$
- c) 7.3 ppm, 2H, triplet, $\text{CH=CH-CH} \times 2$ (Ar) d) 5.4 ppm, 1H, quartet, $\text{CH}_3\text{-CH=C}$
- e) 1.4 ppm, 2H, sextet, $\text{CH}_3\text{-CH}_2\text{-CH}_2$ f) 8.0 ppm, 1H, singlet, C=CH-C (Ar)
- g) 2.1 ppm, 3H, singlet, $\text{CH}_3\text{-C=C}$ or $\text{CH}_3\text{-C=O}$ or $\text{CH}_3\text{-N}$; need context to choose
- h) 6.8 ppm, 2H, doublet, $\text{CH=CH-C} \times 2$ (Ar) i) 0.9 ppm, 6H, doublet, $\text{CH-CH}_3 \times 2$

Exercise 4.12.2:

Identify the errors in the following partial structures:

- a) 3.6 ppm, 2H, triplet, $\text{CH}_2\text{-CH}_2$ the first carbon must be attached to O to have a shift at 3.6 ppm
- b) 2.1 ppm, 2H, singlet, $\text{CH}_3\text{-C=C}$ the integral says only 2H, not 3H
- c) 7.4 ppm, 2H, doublet, $\text{CH=CH}_2\text{-C}$ the shift implies aromatic, so there can only be one H per carbon; must be symmetry
- d) 1.8 ppm, 2H, quintet, $\text{CH}_2\text{-CH}_4$ there can't be four hydrogens on one carbon; must be some hydrogens on each side
- e) 7.8 ppm, 1H, triplet, -CH=CH_2 the shift implies aromatic, so there can only be one H per carbon; must be one on each side
- f) 1.7 ppm, 1H, nonet, $\text{NH}_2\text{-CH(CH}_3)_2$ an attached nitrogen would shift this hydrogen past 2 ppm; also, coupling is rarely seen across O or N, so the two neighbouring H on the left are probably on a carbon

Exercise 4.13.1:

- a) TBME b) acetone c) THF d) methanol e) ethyl acetate

Exercise 4.14.1:

- a. appearance of CH-O near 3.5 ppm (multiplet, 1H)
- b. appearance of $\text{CH}_2\text{-O}$ near 3.5 ppm (triplet, 2H); disappearance of $=\text{CH}$ near 5-6 ppm (multiplets, total 3H)
- c. appearance of HC=O near 10 ppm (triplet, 1H); disappearance of $=\text{CH}$ near 5-6 ppm (multiplets, total 3H)
- d. appearance of HC=O near 10 ppm (triplet, 1H); disappearance of $\text{CH}_2\text{-O}$ near 3.5 ppm (doublet, 2H)
- e. appearance of $\text{CH}_2\text{-O}$ near 3.5 ppm (triplet, 2H)
- f. appearance of $\text{CH}_2\text{-O}$ near 4 ppm (triplet, 2H)
- g. appearance of $=\text{CH}$ near 5-6 ppm (multiplets, total 2H); disappearance of HC=O near 10 ppm (triplet, 1H);
- h. disappearance of $=\text{CH}$ near 5-6 ppm (multiplets, total 2H); appearance of triplet:sextet:triplet pattern between 1-2 ppm
- i. appearance of HC=O near 10 ppm (triplet, 1H); disappearance of $\text{CH}_2\text{-O}$ near 3.5 ppm (doublet, 2H)
- j. appearance of CH-O near 3 ppm (singlet, 3H) and 3.5 ppm (sextet, 1H); disappearance of $=\text{CH}$ near 5-6 ppm (multiplets, total 2H)

Exercise 4.15.1:

a) student 1: Let's use the $\text{H}_2\text{C-O}$ peak of ethyl propanoate at 4 ppm and the acetonitrile methyl at 2 ppm. The ratio appears to be 2:1, but they represent 2 protons and 3 protons, respectively. That means the ratio of molecules is $2/2:1/3 = 3:1$ ethyl propanoate : acetonitrile.

student 2: We'll use the $\text{H}_2\text{C-O}$ peak of ethyl propanoate at 4 ppm and the $\text{H}_2\text{C-O}$ peak of THF at 3.5 ppm. The ratio appears to be 3:2, but they represent 2 protons and 4 protons, respectively. That means the ratio of molecules is $3/2:2/4 = 12:4 = 3:1$ ethyl propanoate : THF.

student 3: Look at the H_2CCl_2 peak of dichloromethane at 5 ppm and the $\text{H}_2\text{C-O}$ peak of THF at 4 ppm. The ratio appears to be 1:2, and they both represent 2 protons, so the ratio of molecules is 1:2 dichloromethane : ethyl propanoate.

b) student 1: The sample is $\frac{1}{1+3} \times 100\% = 25\%$ acetonitrile.

student 2: The sample is $\frac{1}{1+3} \times 100\% = 25\%$ THF.

student 3: The sample is $\frac{1}{1+2} \times 100\% = 33\%$ acetonitrile.

Exercise 4.15.2:

The obvious NMR handles are the H-C=O aldehyde proton at 10 ppm for benzaldehyde and the alcohol-adjacent H-C-O proton at 4.5 ppm for 1-phenylpropanol.

Each of those peaks represents one proton, so the integral ratio of 1:2 suggests a ratio of benzaldehyde to 1-phenylpropanol of 1:2. That translates into 33% benzaldehyde, 67% 1-phenylpropanol.

Exercise 4.15.3:

The NMR handles here are the H-C=O aldehyde proton at 10 ppm for benzaldehyde and the alcohol-adjacent $\text{H}_2\text{C-O}$ protons near 5 ppm for benzyl alcohol.

In this case, we need to correct for the differing numbers of protons represented by each peak: 1H for the aldehyde peak but 2H for the alcohol one. The integral ratio of 1:6 therefore suggests a ratio of benzaldehyde to 1-phenylpropanol of 1:3. That translates

into 25% benzaldehyde, 75% 1-phenylpropanol.

Exercise 4.15.4:

We could use the peak corresponding to the O-CH-C=O proton above 5 ppm for the repeat unit and the peak for the CH₂-O proton in the initiator/end group near 3.5 ppm. The integral ratio is 24:1, but they represent different numbers of hydrogens, so the repeat unit to end group ratio is really 24/1:1/2, or 48:1. The degree of polymerization is 48.

This page titled [4.18: Solutions to Selected Problems](#) is shared under a [CC BY-NC 3.0](#) license and was authored, remixed, and/or curated by [Chris Schaller](#) via [source content](#) that was edited to the style and standards of the LibreTexts platform.