

3.11: Solutions for Selected Problems

Exercise 3.3.1:

- a) C-H shows up at higher wavenumber, because H is lighter than O
- b) C=O shows up at higher wavenumber, because a double bond is stronger than a single
- c) C \equiv N shows up at higher wavenumber, because a triple bond is stronger than a double
- d) N-H shows up at higher wavenumber, because H is lighter than O
- e) Covalent O-H shows up at higher wavenumber, because a covalent bond is stronger than a hydrogen bond

Exercise 3.4.1:

A C_{sp}²-H bond is stronger than a C_{sp}³-H bond.

Exercise 3.4.2:

The electronegative atom would polarize the nearby C=C bond. The C=C peak in the IR spectrum would become more intense; it might be a medium-sized peak instead of a weak one.

Exercise 3.4.3:

- a) In the terminal alkene, in which the double bond was at the end of the chain, there were two oop bends showing at 900 and 1000 cm⁻¹. In the internal, *cis*-alkene, a single oop bend shows near 700 cm⁻¹.
- b) In the *cis*-alkene, a single oop bend shows near 700 cm⁻¹. In the *trans*-alkene, that single oop bend shifts closer to 1000 cm⁻¹.
- c) 1-octene: two IR bands, near 900 and 1000 cm⁻¹.
cis-2-hexene: one IR bands, near 700 cm⁻¹.
trans-2-hexene: one IR band, near 1000 cm⁻¹.

Exercise 3.4.4:

A CH₂ or H-C-H bending mode involves three atoms: two hydrogens and a carbon. A C=C-H oop bend also involves three atoms: two carbons and a hydrogen. The reduced mass of the atoms involved in the oop bend is greater than the reduced mass of the atoms involved in the CH₂ bend. The oop bend shows up at a lower frequency.

Exercise 3.4.5:

The peak at 3300 cm⁻¹ is in the same region as C-H stretching peaks in other spectra. This peak must correspond to a C_{sp}-H stretch. A C_{sp}-H bond is a little stronger than either a C_{sp}²-H or a C_{sp}³-H bond, so the peak shows up at higher wavenumber.

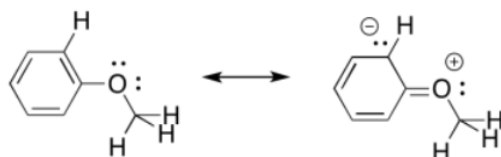
The peak at 2100 cm⁻¹ is not very strong. It corresponds to a relatively non-polar C \equiv C bond. It is a stronger bond than a C=C bond, and so it shows up at higher frequency; the C=C bond would show up around 1600 cm⁻¹. It is also stronger than a C-C bond, which would show up around 1000 cm⁻¹ (although peaks from C-C stretch are very weak and seldom noticed in the spectrum).

Exercise 3.5.1:

The C-O bond is much more polar than the C-H bond. More polar bonds absorb IR light much more strongly than less polar or nonpolar ones.

Exercise 3.5.2:

- a) These peaks correspond to C-O stretches.
- b) There are two distinguishable C-O bonds: one is a C_{sp}²-O bond between the oxygen and the aromatic; the other is a C_{sp}³-O bond between the oxygen and the aliphatic methyl group.
- c) The bond to the aromatic has some double bond character because of conjugation.



d) The partial double bond character means the C_{sp^2} -O bond is a little stronger than the C_{sp^3} -O bond and so the C_{sp^2} -O bond shows up at a higher frequency.

Exercise 3.7.1:

There are actually two N-H stretching bands near 3400 and 3300 cm^{-1} . This feature is common in NH_2 groups; NH groups display only one N-H stretching band.

Exercise 3.7.2:

There is just one N-H stretching band near 3300 cm^{-1} .

Exercise 3.7.3:

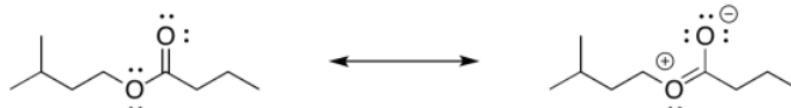
This tertiary amine has no N-H bonds. No N-H stretching frequency would appear in the IR spectrum.

Exercise 3.7.4:

The $C\equiv N$ stretching frequency of the nitrile is visible near 2200 cm^{-1} . In addition, $C=C$ -H oop bends from the aromatic group are visible below 1000 cm^{-1} . The peaks near 1500 cm^{-1} are likely due to $C=C$ stretching; these peaks are more prominent than usual because of polarization by the nitrile, which is a π -acceptor. They are also at slightly low frequency because of the delocalized character of the aromatic double bonds.

Exercise 3.8.1:

The C_{sp^2} -O bond is conjugated, so there is some double bond character, making the bond stronger and moving the IR peak to higher frequency.



Exercise 3.8.2:

OH: 3400 cm^{-1} (strong, broad)

C=O: 1700 cm^{-1} (strong)

C-O: 1050 cm^{-1} (strong)

Exercise 3.10.1:

i. a) O-H b) sp^3 C-H c) C-O

ii. a) sp^2 C-H b) sp^3 C-H c) C=C-H (oop bend)

iii. a) N-H (two of them) b) C=O c) C-N

iv. a) sp^3 C-H b) H-C-H (CH_2 bend)

v. a) sp^3 C-H b) C=O c) H-C-H (CH_2 bend)

vi. a) sp C-H b) sp^3 C-H c) $C\equiv C$

vii. a) N-H b) sp^3 C-H

viii. a) C=O b) C-O

ix. a) N-H (two of them) b) sp^3 C-H

x. a) sp^3 C-H b) aldehyde C-H c) C=O

- xi. a) H-C-H (CH_2 bend) b) C-O
xii. a) O-H (very broad in CO_2H) b) sp^3 C-H c) C=O d) C-O
xiii. a) sp^2 C-H b) sp^3 C-H c) aromatic overtones d) C=C

Exercise 3.10.2:

- a) The rounded OH peak near 3300 cm^{-1} and the strong C-O peak near 1100 cm^{-1} suggest an alcohol.
b) The sharp CH peaks below 3000 cm^{-1} , the weak CH_2 bending modes near 1500 cm^{-1} and the absence of any other features suggest an alkane.
c) The strong C=O peak near 1700 cm^{-1} and the strong C-O peak near 1100 cm^{-1} suggest an ester.
d) The strong C=O peak near 1700 cm^{-1} and the absence of additional features other than those associated with saturated hydrocarbons suggest a ketone.
e) The CH peak above 3000 cm^{-1} and the strong oop bending modes below 1000 cm^{-1} suggest an alkene. The presence of two oop bending peaks may point to a terminal alkene ($\text{C}=\text{CH}_2$).
f) The sharp N-H peaks near 3200 cm^{-1} and the strong C=O peak near 1600 cm^{-1} suggest an amide. The presence of two N-H peaks rather than one points to a primary amide ($\text{O}=\text{C}-\text{NH}_2$).
g) The small, triangular "sharktooth" peak near 3200 cm^{-1} suggests an amine. With just one N-H peak, this is probably a primary amine ($\text{R}-\text{NH}_2$).
h) The strong C-O peak near 1100 cm^{-1} suggests an ether.
i) The C-H peaks above 3000 cm^{-1} and the oop bending modes below 1000 cm^{-1} certainly suggest double bonds. The progression of tooth-like "aromatic overtones" between 1600 and 2000 cm^{-1} strongly indicates a substituted benzene.
j) The small, triangular "sharktooth" peaks near 3200 cm^{-1} suggest an amine. With two N-H peaks, this is probably a secondary amine (R_2NH).
l) The broad, deep OH peak between 3300 cm^{-1} and 2600 cm^{-1} and the C=O peak near 1700 cm^{-1} suggests a carboxylic acid. The O-H peak of a carboxylic acid is often missed; it is moved to lower frequency by hydrogen bonding.

Exercise 3.10.3

- i)
a)
 3200 cm^{-1} (sharp): N-H
 2900 cm^{-1} (sharp): $\text{C}_{\text{sp}^3}\text{-H}$
 1600 cm^{-1} (broad): probably NH_2 bending
b) A primary amine.
c)
ii)
a)
 3400 cm^{-1} (strong, broad): O-H
 2900 cm^{-1} (sharp): $\text{C}_{\text{sp}^3}\text{-H}$
 1050 cm^{-1} (strong): probably C-O
b) Alcohol.
c)
iii)
a)

2900 cm^{-1} (sharp): $\text{C}_{\text{sp}^3}\text{-H}$

1700 cm^{-1} (strong): C=O

1200 and 1000 cm^{-1} (strong & medium): C-O

b) Ester

c)

iv)

a)

3050 cm^{-1} (sharp): $\text{C}_{\text{sp}^2}\text{-H}$

1700 cm^{-1} (strong): C=O

1200 and 1000 cm^{-1} (strong & medium): C-O

b) Ester; probably contains an aromatic as well

c)

v)

a)

2750 and 2650 cm^{-1} (medium, sharp): C-H of an aldehyde

1700 cm^{-1} (strong): C=O

Below 1000 cm^{-1} (strong & medium): oop bends

b) Aldehyde; probably contains an aromatic as well

c)

Problem 3.10.4

Problem 3.10.5

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