Answers to IR Handout

#1. Ignore peaks below 1600 cm\(^{-1}\). This is the finger print region and while it contains much useful information it is difficult to interpret without more experience.

What are the major (strong) absorptions above 1600 cm\(^{-1}\)?

A set of peaks at about 3000 cm\(^{-1}\).

What functional group is indicated by these peaks?

Peaks at about 3000 cm\(^{-1}\) corresponds to various C–H stretching vibrations (modes). This molecule appears to have only the alkane as a functional group.

The mass spec indicates 8 C’s: ratio of M+1 to M\(^+\) abundances (expressed as %) ÷ 1.1 % (the natural abundance of 13C) = # of C’s, i.e. 8.8 ÷ 1.1 = 8 C’s. Note this rule does not always work.

C\(_8\) has a mass of 96. Since the MW = 114 according to the parent peak, the remaining mass is 18. Initial guess is therefore C\(_8\)H\(_{18}\). This molecule is fully saturated. One possible structure is:

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#2. Again ignore the fingerprint region below 1600 cm\(^{-1}\).

What are the major (strong) absorptions above 1600 cm\(^{-1}\)?

First ignore the peaks at 1800 cm\(^{-1}\) and 1950 cm\(^{-1}\). They are weak and difficult to interpret. However there is a set of strong peaks at about 3000 cm\(^{-1}\).

What functional group is indicated by these peaks?

No other major peaks are seen so this is probably a hydrocarbon of some sort.

Careful inspection of the peaks indicate that they are all just above 3000 cm\(^{-1}\). As a general rule C–H vibrations above 3000 are seen when the C is sp\(^2\) (or sp) hybridized; on the other hand C–H vibrations just below 3000 cm are seen when the C is sp\(^3\) hybridized. We conclude the molecule contains sp\(^2\) C, i.e. at least one \(\pi\) bond and one degree of unsaturation.

The MS shows a parent peak at 78 and therefore a MW of 78. The abundance of the M+1 indicates there should be 6 C’s (6.6 ÷ 1.1 = 6). Six Cs has a mass of 72. That leaves 6 Hs. A likely MF is C\(_6\)H\(_6\). This shows 4\(^\circ\) unsaturation, which is consistent with the presence of \(\pi\) bonds seen in the IR.

A possible structure consistent with this is benzene:
#3. What are the major (strong) absorptions above 1600 cm$^{-1}$?

The usual set of peaks at about 3000 cm$^{-1}$ (actually below 3000 cm$^{-1}$, therefore no H on $sp^2$ Cs). Additionally there is a strong peak at about 1700 cm$^{-1}$.

What functional group is indicated by these peaks?

Peaks around 1700 cm$^{-1}$ are indicative of the carbonyl, C=O. Therefore not only oxygen present, there is at least one degree of unsaturation.

From the MS data we know the MW is 86 (from the parent peak). 86 – 16 (atomic mass of oxygen) = 70. What has a mass of 70? Probably something with 5 Cs. 70 – 5x12 = 10, so it's likely that 10 Hs are present. This gives C$_5$H$_{10}$O, which has one degree of unsaturation, as predicted by the C=O. A possible structure is a ketone such as

\[ \text{CH}_5 \text{C} = \text{O} \text{CH}_3 \]

Note the exact position of the C=O is at 1717 cm$^{-1}$. You will later learn that this is consistent with ketone, but not aldehyde.

#4. What are the major (strong) absorptions above 1600 cm$^{-1}$?

The usual set of peaks at about 3000 cm$^{-1}$ (actually below 3000 cm$^{-1}$, therefore no H on $sp^2$ Cs). Additionally there is a strong, noticeably broad peak at about 3350 cm$^{-1}$.

What functional group is indicated by these peaks?

Broad peaks around 3400 cm$^{-1}$ are indicative of the O–H stretching vibration of the hydroxy group. Thus an alcohol is indicated. Oxygen is present. Since the hydroxy group has only single bonds, this functional group contributes no degrees of unsaturation.

From the MS data we know the MW is 74 (from the parent peak). 74 – 16 (atomic mass of oxygen) = 58. What has a mass of 58? Probably something with 4 Cs. 58 – 4x12 = 10, so it's likely that 10 Hs are present. This gives C$_4$H$_{10}$O, which is fully saturated (2n+2 Hs) and is consistent with the IR frequencies. A possible structure is an alcohol such as

\[ \text{CH}_4 \text{OH} \]

#5. What are the major (strong) absorptions above 1600 cm$^{-1}$?

The usual set of peaks at about 3000 cm$^{-1}$ (actually below 3000 cm$^{-1}$, therefore no H on $sp^2$ Cs). Additionally there is a strong peak about 1700 cm$^{-1}$.

What functional group is indicated by these peaks?

The peak around 1700 cm$^{-1}$ indicates a carbonyl C=O. Subtle distinctions between the different types of carbonyls can be made. For example we have previously seen (#3) that peaks around 1705 – 1715 cm$^{-1}$ are indicative of ketones. Peaks at the higher end (around 1740 cm$^{-1}$) are more likely to be esters: RC(=O)OR. Thus two oxygens and at least one degree of unsaturation is expected.
From the MS data we know the MW is 88 (from the parent peak). 88 – 2x16 (atomic mass of oxygen) = 56. What has a mass of 56? Probably something with 4 Cs. 56 – 4x12 = 8, so it is likely that 8 Hs are present. This gives \( \text{C}_4\text{H}_8\text{O}_2 \), which contains one degree of unsaturation and is thus consistent with conclusions from the IR. A possible structure is an ester such as

\[
\text{C}_4\text{H}_8\text{O}_2
\]

**#6.** What are the major (strong) absorptions above 1600 cm\(^{-1}\)?

There is a set of peaks about 3000 cm\(^{-1}\) but they are not as sharp as usual. In fact the usual set of peaks at about 3000 cm\(^{-1}\) is actually obscured by a strong, very broad peak (much broader than the OH). Additionally there is a strong peak about 1700 cm\(^{-1}\).

What functional group is indicated by these peaks?

Although the C–H vibrations are obscured, it is safe to assume that C–H is present – most organic molecules contain CH bonds. The peak around 1700 cm\(^{-1}\) indicates a carbonyl C=O. The real give-away here is the presence of such exceedingly broad peaks. There is only one functional group that gives such broad peaks that span the range of 2400 – 3400 cm\(^{-1}\): the carboxylic acid: RC(=O)OH. Thus two oxygens and at least one degree of unsaturation is expected.

From the MS data we know the MW is 88 (from the parent peak). 88 – 2x16 (atomic mass of oxygen) = 56. What has a mass of 56? Probably something with 4 Cs. 56 – 4x12 = 8, so it is likely that 8 Hs are present. This gives \( \text{C}_4\text{H}_8\text{O}_2 \), which contains one degree of unsaturation and is thus consistent with conclusions from the IR. A possible structure is a carboxylic acid such as

\[
\text{C}_4\text{H}_8\text{O}_2
\]

**#7.** What are the major (strong) absorptions above 1600 cm\(^{-1}\)?

The peaks around 3000 cm\(^{-1}\) are unusually weak. This is an indication that the Hs are on \( sp^2 \) Cs. Additionally there is a strong peak about 1700 cm\(^{-1}\).

What functional group is indicated by these peaks?

Although the C–H vibrations are weak, it is safe to assume that C–H is present – most organic molecules contain CH bonds. The peak around 1700 cm\(^{-1}\) indicates a carbonyl C=O. Thus oxygen and at least one degree of unsaturation are indicated.

From the MS data we know the MW is 106 (from the parent peak). 106 – 16 (atomic mass of oxygen) = 90. What has a mass of 90? Probably something with 7 Cs. 90 – 7x12 = 6, so it is likely that 6 Hs are present. This gives \( \text{C}_7\text{H}_6\text{O} \), which contains five (!) degrees of unsaturation and is thus consistent with conclusions from the IR. This is a lot of unsaturation for such a small molecule. Whenever 4 or more degrees of unsaturation are present, a benzene ring becomes likely. Benzene has four degrees of unsaturation (3 \( \pi \) bonds + one ring). Combining information (benzene ring + C=O) leads to only one structure (that does violate carbons tetravalency):
Note that the aldehydic C–H stretch is unusual – not only is it weak, but it also is seen as a pair of peaks at about 2750 and 2850 cm\(^{-1}\).

#8. What are the major (strong) absorptions above 1600 cm\(^{-1}\)?

The peaks around 3000 cm\(^{-1}\) are unusually weak. This is an indication that the Hs are on \(sp^2\) Cs. Additionally there is a strong peak about 2200 cm\(^{-1}\).

What functional group is indicated by these peaks?

Although the C–H vibrations are weak, it is safe to assume that C–H is present – most organic molecules contain CH bonds. The peak around 2200 cm\(^{-1}\) can only be one functional group, the nitrile \(-\text{C.triplebond.N.}\)

From the MS data we know the MW is 53 (from the parent peak). The odd MW indicates N is present and this is consistent with nitrile (CN) observed in the IR. \(53 - (12 + 14)\) (atomic mass of carbon & nitrogen) = 27. What has a mass of 27? Probably something with 2 Cs. \(27 - 2 \times 12 = 3\), so it is likely that 3 Hs are present. This gives \(\text{C}_3\text{H}_3\text{N}\), which clearly contains some degrees of unsaturation although our previous rules for assigning degrees of unsaturation don’t work because N is trivalent. For just two Cs and 3 Hs one comes by trial and error to:

\[\equiv\text{N}\]