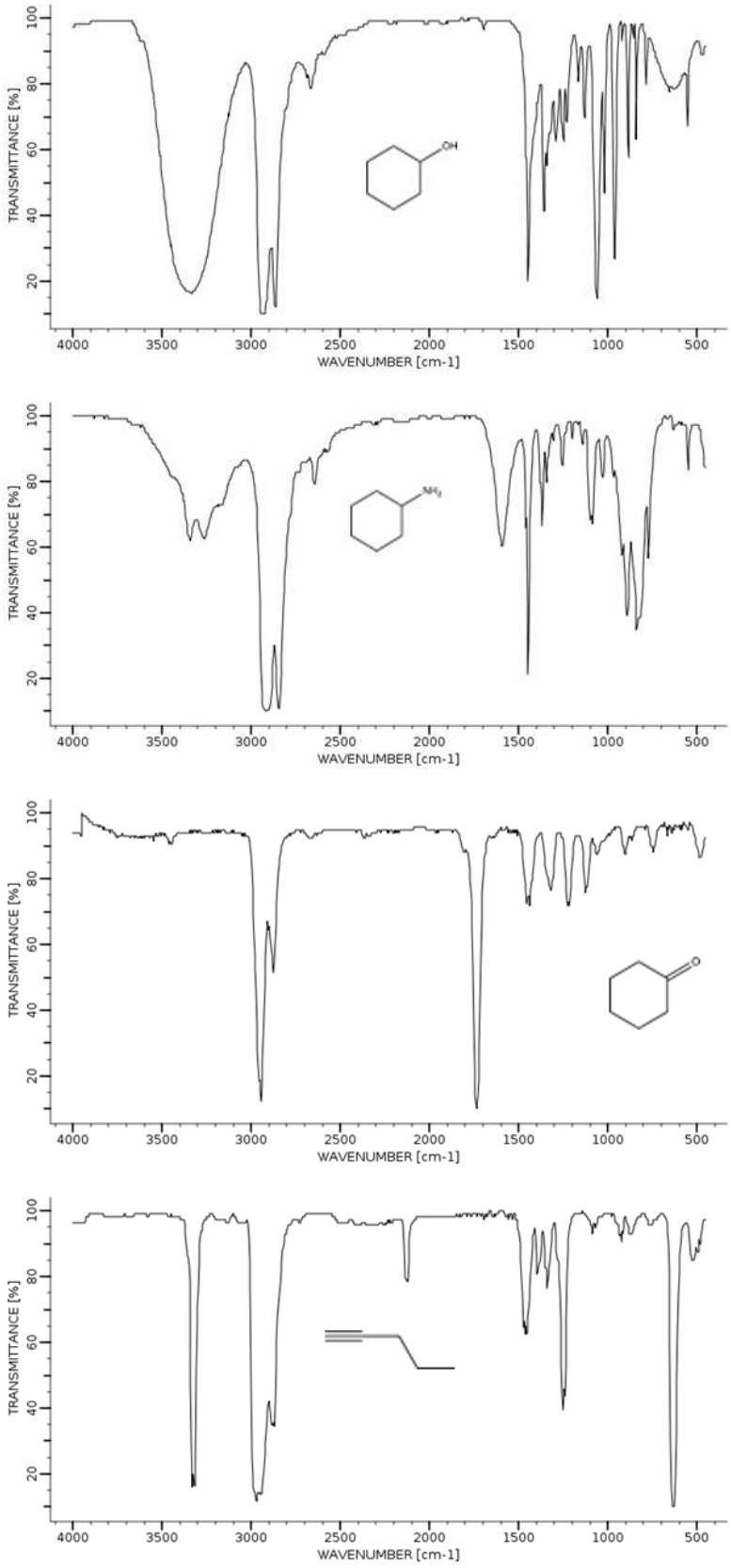
CHEM1102 Worksheet 4 – Answers to Critical Thinking Questions

The worksheets are available in the tutorials and form an integral part of the learning outcomes and experience for this unit.

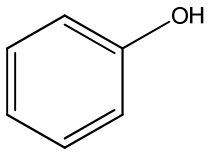
Model 1: Infrared (IR) Spectroscopy

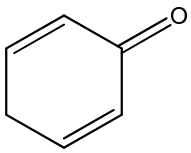
1. See below.

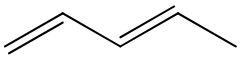
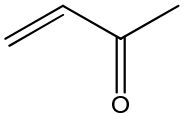


Model 2: UV-Visible Spectroscopy

1. See below.



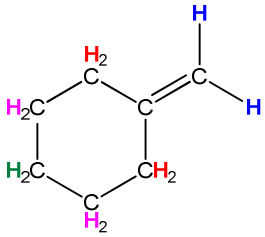


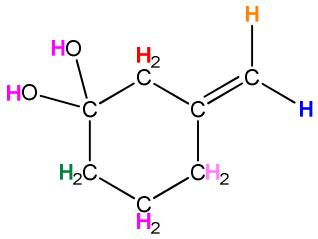



2. All of the above.
3. Restricted to the identification of conjugation.

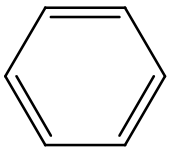
Model 3: ^{1}H NMR Spectroscopy - Chemical Shifts

1. The molecule on the left has 4 types of H atom and the molecule on the right has 7 types of H atom*.

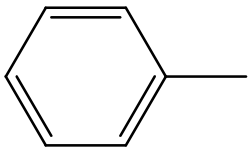




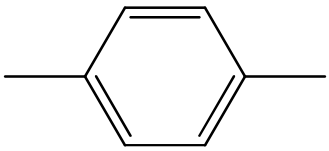
2. The molecule on the left will give 4 signals and the molecule on the right will give 7 signals.
3. See below.



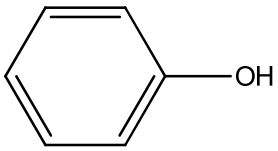
1 signal – between 6.5 – 8.0 ppm due to ArH



4 signals – one at 2 - 3 ppm (-CH_3) and three between 6.5 and 8.0 ppm (ArH).



2 signals – one at > 2 ppm (-CH_3) and one between 6.5 and 8.0 ppm (ArH)



4 signals – one between 4.0 and 8.0 ppm (-PhOH) and three between 6.5 and 8.0 ppm (ArH)

Model 4: ^{1}H NMR Spectroscopy - Coupling

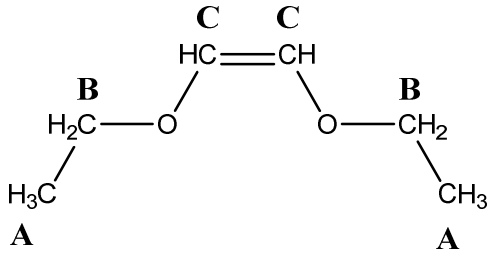
1. Number of peaks = n + 1 where n is the number of hydrogen atoms on adjacent atoms which are not equivalent to the ^{1}H giving rise to the signal.
2. None.
3. A septet with intensity ratio 1: 6 : 15 : 20 : 15 : 6 : 1.

Model 5: ^{1}H NMR Spectroscopy - Integration

1. There are 3 signals due to the 3 types of ^{1}H environment: A, B and C.

* The ring in these two molecules is not planar. You might like to re-consider these answers taking into account the 3D structure

The signal at 1.3 ppm is due to the 6 ^{1}H in environment A: integral = 6. The signal is split into a 1:2:1 triplet due to coupling to the 2 ^{1}H on the neighbouring CH_2 group (B).

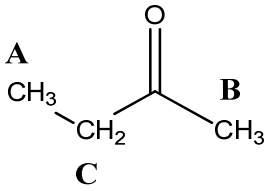


The signal at 4.5 ppm is due to the 4 ^{1}H in environment B: integral = 4. The signal has a higher chemical shift than that for group A due to the presence of the electronegative O atom. The signal is split into a 1:3:3:1 quartet due to coupling to the 3 ^{1}H on the neighbouring CH_3 group (A).

The signal at ~5.3 ppm is due to the 2 ^{1}H in environment C: integral = 2. The signal has a higher chemical shift than that for group A or B as the ^{1}H atoms are on a sp^2 C atom that is bonded to an electronegative O atom. There are no ^{1}H on the neighbouring atoms, except the other equivalent ^{1}H atom, so no splitting due to coupling is observed.

2. There are 3 signals due to the 3 types of ^{1}H environment: A, B and C.

The signal at ~1.1 ppm is due to the 3 ^{1}H in environment A: integral = 2. The signal is split into a 1:2:1 triplet due to coupling to the 2 ^{1}H on the neighbouring CH_2 group (C).



The signal at 2.1 ppm is due to the 3 ^{1}H in environment B: integral = 3. The signal has a higher chemical shift than that for group A due to the presence of the electronegative O atom. There are no ^{1}H on the neighbouring atoms, so no splitting due to coupling is observed.

The signal at ~2.5 ppm is due to the 2 ^{1}H in environment C: integral = 2. The signal has a higher chemical shift than that for group A due to the presence of the electronegative O atom. The signal is split into a 1:3:3:1 quartet due to coupling to the 3 ^{1}H on the neighbouring CH_3 group (A).

3. H_B have the highest shift since they are closest to the electronegative O atoms. There are two H_B atoms so the signal has an integral of 2. The H_B atoms are coupling to 3 × H_C atoms giving rise to a (n + 1) = (3 + 1) = 4 line multiplet (a *quartet*).

H_C have the lowest shift since they are further from the electronegative O atoms. There are three H_B atoms so the signal has an integral of 3. The H_C atoms are coupling to 2 × H_B atoms giving rise to a (n + 1) = (2 + 1) = 3 line multiplet (a *triplet*).