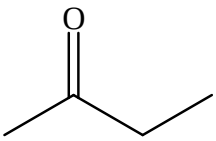
School of Chemistry

Chemistry 1B Advanced and SSP (CHEM1902/1904)

Answers to Problem Sheet 2

1. **The compound is $C_2H_6N_2$.**
Molar masses: C_3H_6O 58.042 g mol^{-1}, C_4H_{10} 58.078 g mol^{-1}, $C_2H_6N_2$ 58.053 g mol^{-1}

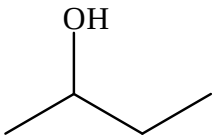
2. (a)



butan-2-one

Low resolution MS: molar mass = 72 g mol^{-1} (C_4H_8O)

IR: ~1700 cm^{-1} for C=O

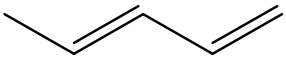


butan-2-ol

Low resolution MS: molar mass = 74 g mol^{-1} ($C_4H_{10}O$)

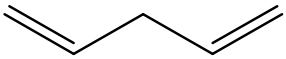
IR: ~3300 cm^{-1} (broad) O-H

(b)



(*E*)-penta-1,3-diene

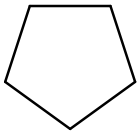
UV: conjugated double bonds leads to strong absorption



penta-1,4-diene

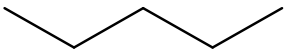
UV: double bonds are not conjugated so no strong absorption

(c)



cyclopentane

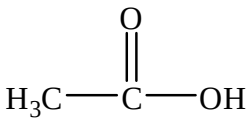
Low resolution MS: molar mass = 70 g mol^{-1} (C_5H_{10})



pentane

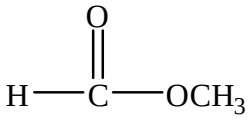
Low resolution MS: molar mass = 72 g mol^{-1} (C_5H_{12})

(d)



acetic acid

IR: ~3300 cm^{-1} (very broad) O-H, ~1700 cm^{-1} C=O

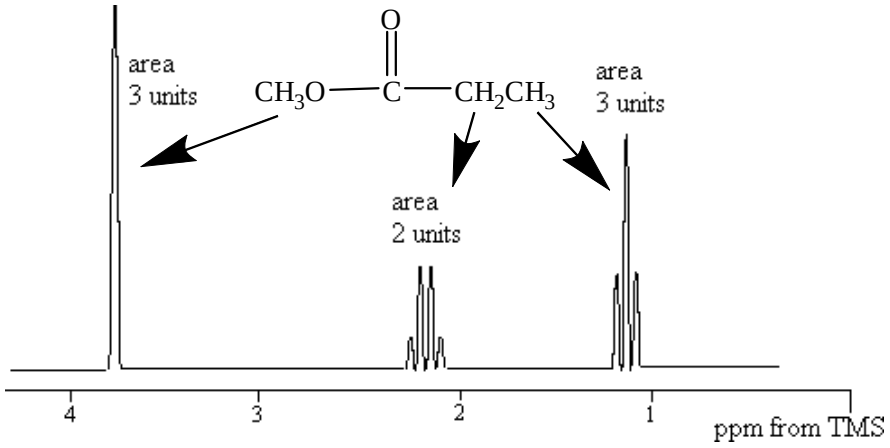


methyl formate

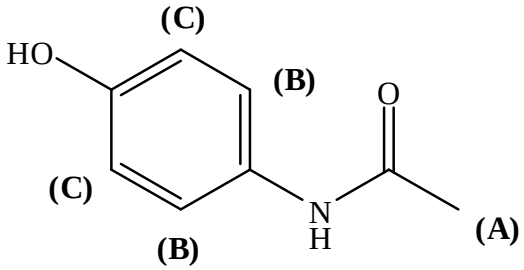
IR: ~1700 cm^{-1} C=O

^{1}H and ^{13}C NMR could be used in all cases.

3. (a) **A, B and C**
(b) **E**
(c) **D**
(d) **2**
(e) **B and C**
(f) **B**



4. **There are three sets of equivalent ^{1}H atoms bonded to carbon in paracetamol:**

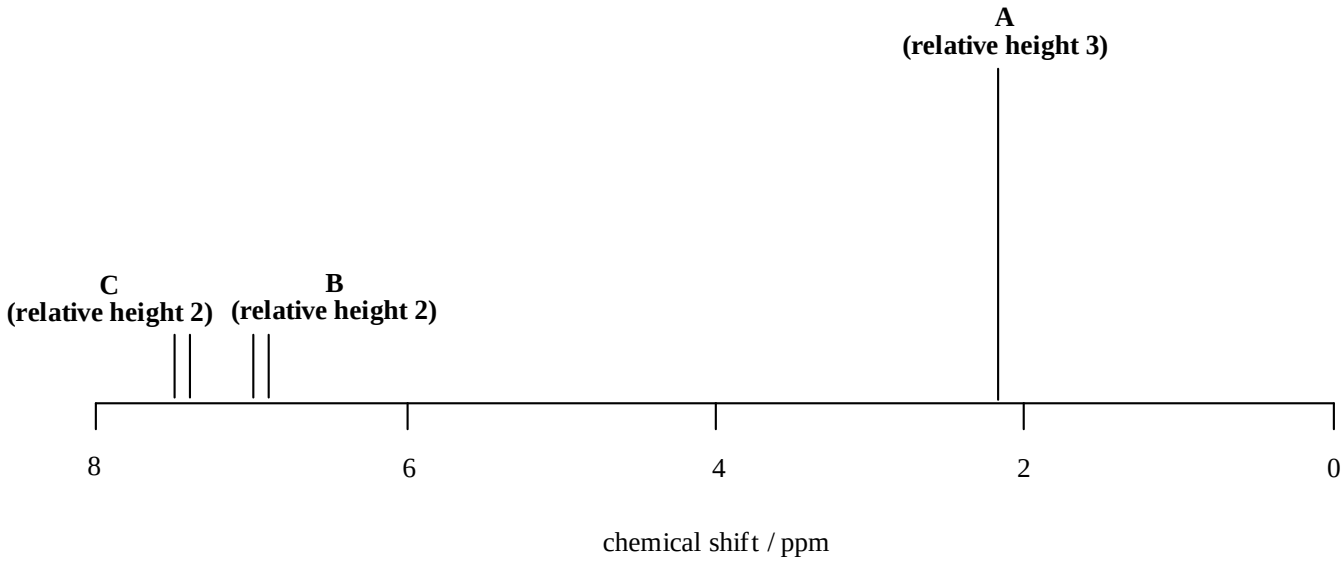


- **(A) corresponds to the three equivalent ^{1}H on a -CH_3 group. These are expected to have a chemical shift of 0.8 – 1.8 ppm. As it is due to three ^{1}H, the signal will have a relative area of 3.**
- **(B) corresponds to two equivalent ^{1}H on the ring. These are expected to have a chemical shift of 6 – 9 ppm. As it is due to two ^{1}H, the signal will have a relative area of 2.**
- **(C) correspond to another two equivalent ^{1}H on the ring. These are expected also to have a chemical shift of 6 – 9 ppm. As it is due to two ^{1}H, the signal will have a relative area of 2.**
- **The chemical shifts of {C} will be different to those of {B} but you are *not* expected to order them.**

Each proton in {B} is adjacent to one proton from set {C} and coupling will split the signal due to the {B} protons into a doublet.

Each proton in {C} is adjacent to one proton from set {B} and coupling will similarly split the signal due to the {C} protons into a doublet.

The ^{1}H NMR spectrum due to the protons bonded to carbon will thus consist of three signals (due to A, B and C) and the signals due to B and C will be doublets.


A
(relative height 3)
C
(relative height 2)
B
(relative height 2)
8
6
4
2
0
chemical shift / ppm