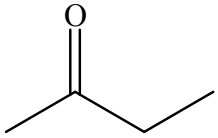
CHEM1102 Answers to Problem Sheet 4

1.

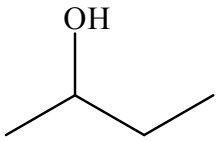
(a)



butan-2-one

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

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

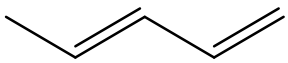


butan-2-ol

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

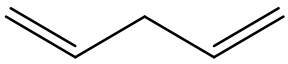
IR: ~3300 cm^{-1} (broad) O-H

(b)



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

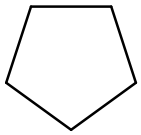
UV: conjugated double bonds leads to strong absorption



penta-1,4-diene

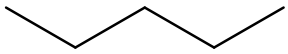
UV: double bonds are not conjugated so no strong absorption

(c)



cyclopentane

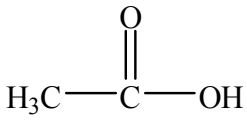
Low resolution MS: molar mass = 70 g mol^{-1} (C_5H_{10})



pentane

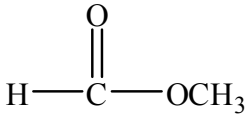
Low resolution MS: molar mass = 72 g mol^{-1} (C_5H_{12})

(d)



acetic acid

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

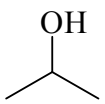


methyl formate

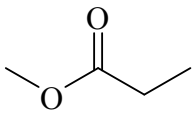
IR: ~1700 cm^{-1} C=O

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

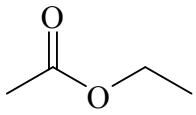
2. .



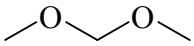
A



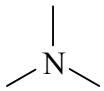
B



C



D



E

(a) **A, B and C would all give three signals in the ^{1}H NMR spectrum**

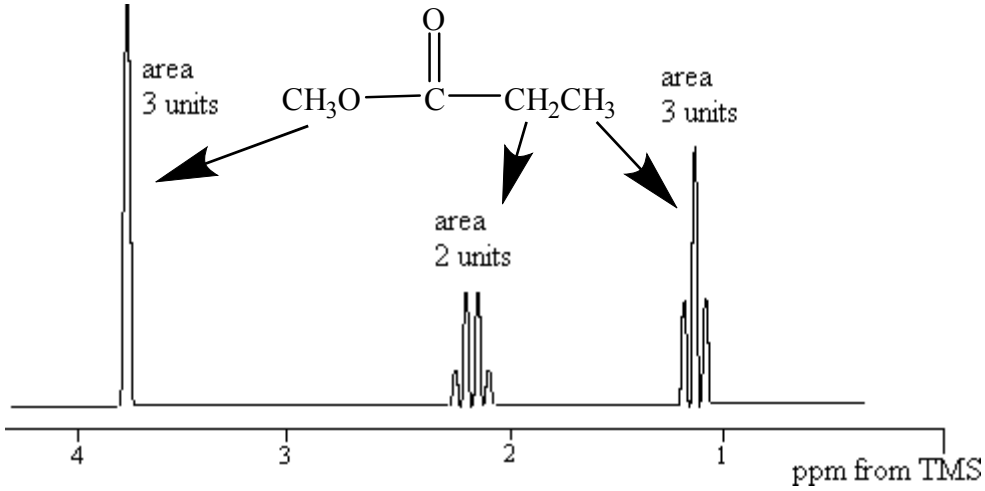
(b) **E possesses a ^{1}H NMR spectrum consisting of only one resonance**

(c) **D possesses a ^{1}H NMR spectrum consisting of two signals in the ratio 1:3**

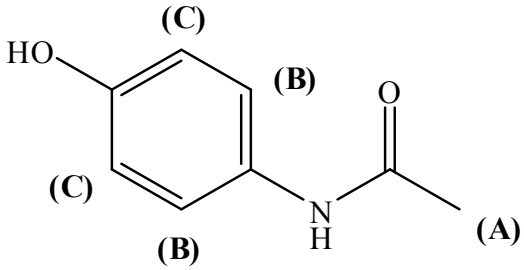
(d) **Two singlets would be observed in the ^{1}H NMR spectrum of D**

(e) **B and C both possess ^{1}H NMR spectra containing a singlet, a triplet and a quartet**

(f) **The ^{1}H NMR spectrum below belongs to B:**



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



- **(A) corresponds to the three equivalent ^1H 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 ^1H, the signal will have a relative area of 3.**

- **(B) corresponds to two equivalent ^1H on the ring. These are expected to have a chemical shift of 6 – 9 ppm. As it is due to two ^1H, the signal will have a relative area of 2.**

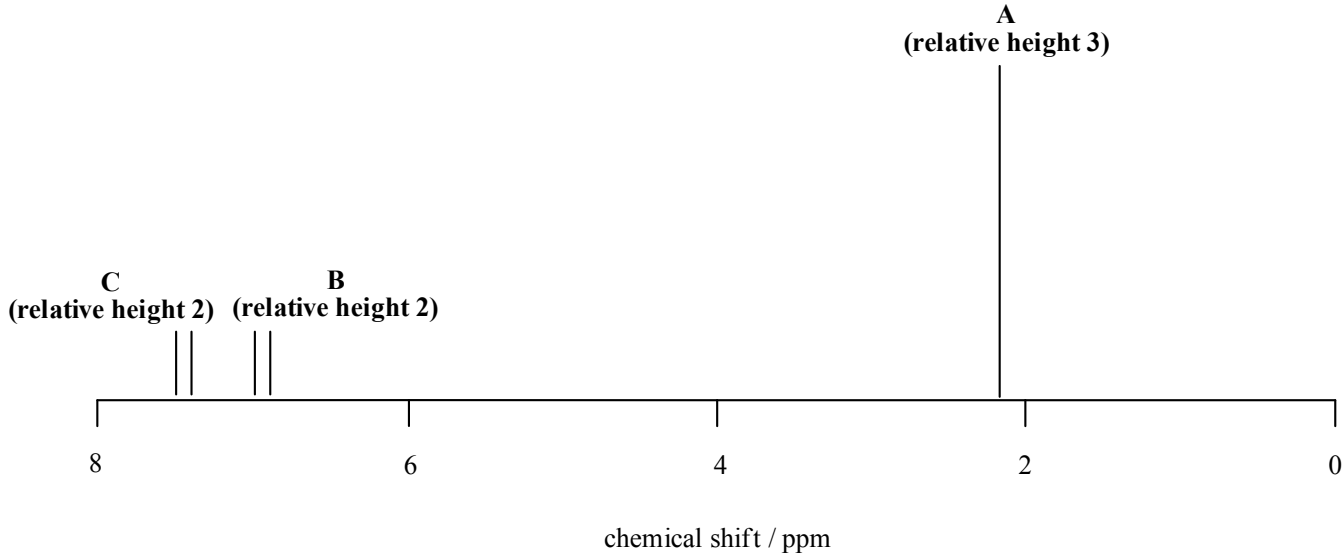
- **(C) correspond to another two equivalent ^1H on the ring. These are expected also to have a chemical shift of 6 – 9 ppm. As it is due to two ^1H, the signal will have a relative area of 2.**

- **The chemical shifts of {C} will be different to those of {B} but you are *not* expected to order them.**

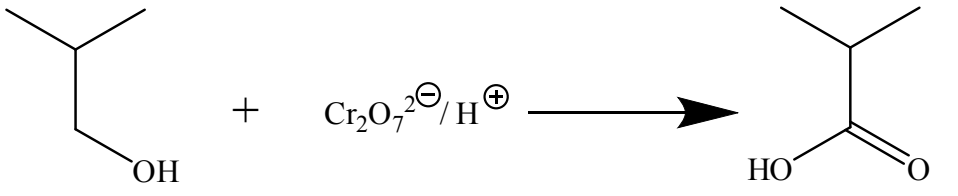
Each proton in {B} is adjacent to one proton from set {C} and coupling will split the signal due to the {B} protons into a doublet.

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 ^1H 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.

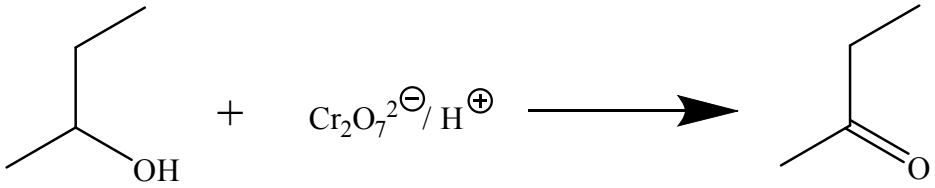


4.



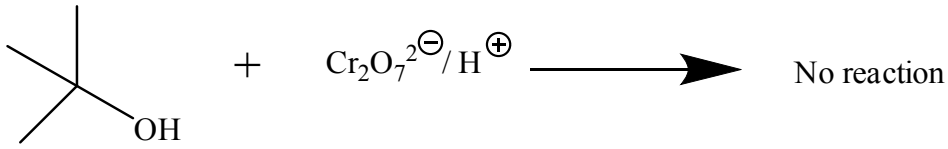
2-methylpropan-1-ol **isobutyric acid**

1° alcohol → carboxylic acid



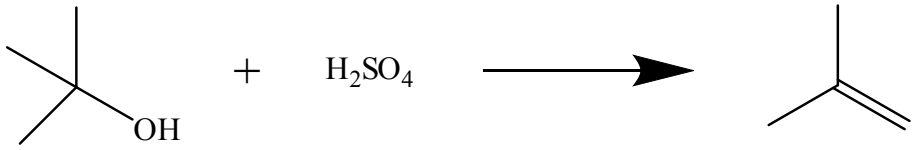
butan-2-ol **butan-2-one**

2° alcohol → ketone



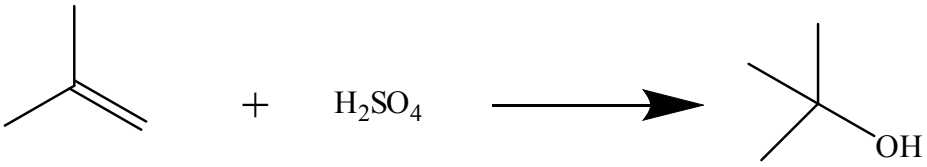
2-methylpropan-2-ol

3° alcohol – no reaction with oxidizing agent



2-methylpropan-2-ol **2-methylprop-1-ene**

Dehydration of 3° alcohol



2-methylprop-1-ene **2-methylpropan-2-ol**

Hydration of a C=C bond

See the 'Organic Spectroscopy' website for more information and practice:
https://scilearn.sydney.edu.au/OrganicSpectroscopy/