CHEM1002 Worksheet 5 – Answers to Critical Thinking Questions

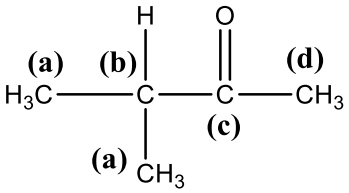
The worksheets are available in the tutorials and form an integral part of the learning outcomes and experience for this unit.

Model 1: Mass Spectrometry

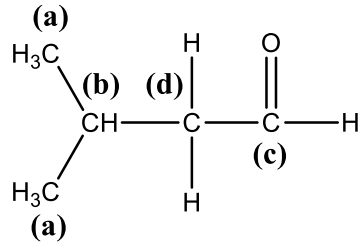
1. Acetonitrile: $CH_3C{\equiv}N$.

Model 2: Combined Use of Mass Spectrometry and IR, UV-Visible and NMR Spectroscopy to Identify Unknown Compounds.

1. The ^{13}C NMR shows 4 peaks due to (a) at 18 ppm, (b) at 42 ppm, (c) at 210 ppm and (d) at 27 ppm. The IR indicates the presence of a C=O group. The molecule is the ketone below:

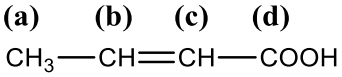


The aldehyde below is also a reasonable fit, although the carbon labelled (b) is too far from the C=O group for its chemical shift to be as high as 42 ppm.

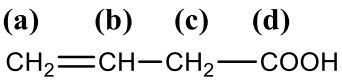


2. The IR indicates the presence of a C=O and a O-H group. There are two possibilities:

   (i) The ^{13}C NMR shows 4 peaks due to (a) at 40 ppm, (b) at 120 ppm, (c) at 130 ppm and (d) at 178 ppm.

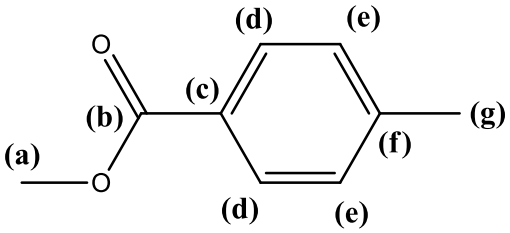


   (ii) The ^{13}C NMR shows 4 peaks due to (a) at 120 ppm, (b) at 130 ppm, (c) at 40 ppm and (d) at 178 ppm.



   UV-Visible spectroscopy could be used to resolve which is correct as (i) contains a conjugated double bond. [The answer is actually (ii).]

3. The ^{13}C NMR shows 7 peaks due to (a) at 52 ppm, (b) at 168 ppm, (c) at 144 ppm, {(d), (e) and (f)} between 128 – 132 ppm and (g) at 22 ppm. The IR indicates the presence of a C=O group.


(d)
(e)
O
(c)
(b)
(g)
(a)
(f)
O
(d)
(e)