Student 1: Excellence

NZQA Intended for teacher use only

The IR spectrum shows 2 medium sized peaks at 2822 cm^{-1} and 2719 cm^{-1} these could be the C=C-H stretch of an aldehyde. There is a strong peak at 1728 cm^{-1} which could be the C=O stretch of an aldehyde. There is another strong peak at 2960 cm^{-1} which could be a C-H stretch. 1

Compound Q cannot be an amine because if it was an amine then I would expect to see a double peak between 3500 cm^{-1} and 3300 cm^{-1} for the N-H stretch, however this isn't present. Also, there is no peak between 1640 cm^{-1} and 1500 cm^{-1} for the N-H bond present. In an amine, we also wouldn't expect to see the strong peak at 1728 cm^{-1}. Therefore, it isn't an amine and so isn't compound 4 or 7. If it was a ketone then I wouldn't expect to see the peaks at 2822 cm^{-1} and 2719 cm^{-1} for the O=C-H stretch. Also, the strong C=O stretch would be a bit lower, between 1720 cm^{-1} and 1715 cm^{-1}. So, it isn't a ketone and therefore compound Q isn't molecule 1,2 or 6. 2

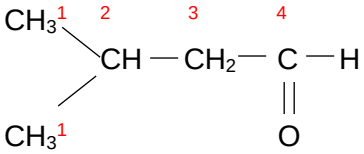
From the peaks shown in the IR spectrum I believe that compound Q is an aldehyde. This is because of the two peaks at 2822 cm^{-1} and 2719 cm^{-1} for the O=C-H stretch and the strong peak at 1728 cm^{-1} for the C=O stretch. Therefore, it is either molecule 3, 5 or 8.

The C-13NMR spectrum shows 4 peaks this means that there are 4 unique carbon environments. Molecule 1 only has 3 unique carbon environments so it can't be this molecule. Molecules 4 and 5 both have 5 unique carbon environments so it can't be these either. Molecules 2, 3, 6, 7 and 8 all have 4 unique carbon environments so compound Q is one of these molecules. However as shown by the IR spectrum compound Q is an aldehyde so the compound will either be molecule 3 or 8.

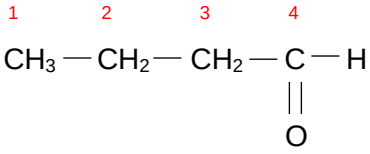
There is a peak at 22.59 ppm which could be a CH_3 carbon. There is another peak at 23.57 ppm which could be a CH carbon or a CH_2 carbon. There is another peak at 52.66 ppm this is the CH_2 carbon which has been downshifted because it is bonded to the functional group. There is another peak at 202.71 ppm this is the C=O carbon of the aldehyde. These peaks show that compound Q is an aldehyde with 4 unique carbon environments so therefore compound Q is either molecule 3 or 8. 1

If it was an amine the I would expect to see a peak between 70 ppm and 30 ppm. A peak is present in that region but I wouldn't expect to see a peak at 202.71 ppm, so it cannot be an amine and therefore not molecule 4 or 7. If it was a ketone then I would have expected to see the peak at 202.71 ppm a bit more downstream and shown in the IR spectrum it isn't a ketone. 2

Molecule 3



Molecule 8



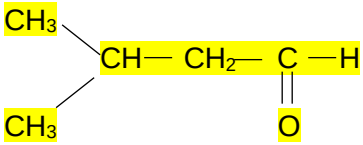
Both compounds have 4 unique carbon environments and are both aldehydes.

Molar mass =
(5x12) + (10x1) + 16 = 86 g mol^{-1}

Molar mass =
(4x12) + (8x1) + 16 = 72 g mol^{-1}

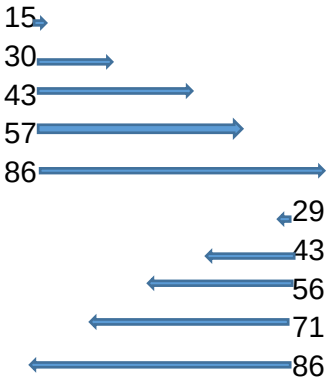
The mass spectrum shows that compound Q has a molecular ion peak of 86m/z which is means that mass of the compound is 86 g mol^{-1}. This means that compound Q could be molecule 1, 2, 3, or 5 as they all have a molar mass of 86 g mol^{-1}. Molecule 4 and 7 both have a molar mass of 87 g mol^{-1} so it can't be them. Molecule 6 and 8 both have a molar mass of 72 g mol^{-1} so it can't be them either. 1

86 g mol^{-1} is an even number therefore there is either an even number of nitrogens present or zero nitrogens present. This means compound Q cannot be molecule 4 or 7, as they are both amines which have 1 nitrogen and have a molar mass of 87 g mol^{-1} which is an odd number. The IR and C-13NMR spectrum showed that the molecule was either molecule 3 or 8 so because molecule 8 has a molar mass of 72 g mol^{-1} compound Q must be molecule 3. 2



3

The expected fragments on the mass spectrum for molecule 3 are:
CH_3 / CH_3 / CH / CH_2 / COH



There is a peak at 29 m/z for the COH^+ fragment and another peak at 15 m/z for the CH_3^+ fragment. There is a peak at 43 m/z which could be the $CH_3CH_3CH^+$ or CH_2COH^+ fragment. There is another peak at 71 m/z which is the $CH_3CHCH_2COH^+$ fragment. There is a peak at 86 m/z which is the molecular ion peak for $CH_3CH_3CHCH_2COH^+$. These peaks all confirm that compound Q is molecule 3 as they can form from the structure as shown above.

Shown by the IR spectrum, C-13NMR and mass spectrum I have found that compound Q is molecule 3. It is an aldehyde with a molar mass of 86 g mol^{-1} and 4 unique carbon environments. 3

Because it is molecule 3 this means that on the C-13NMR spectrum the peak 22.59 ppm is the CH_3 carbon, the peak at 23.57 ppm is the CH carbon, the peak at 52.66 ppm is the downshifted CH_2 carbon and the peak at 202.71 ppm is the C=O carbon of an aldehyde.