Year 13 Science: Spectroscopic data: identifying organic compounds

Name: _____ Date: _____

Try these without your notes first, then check the answer key.

Practice

1. A C_3H_8O alcohol has a broad IR dip at 3350 cm^{-1} and two peaks in its ^{13}C NMR spectrum. Name it.

2. How many peaks does pentan-3-one, $CH_3CH_2COCH_2CH_3$, give in its ^{13}C NMR spectrum?

3. A haloalkane has molecular ion peaks at m/z 78 and 80 in a 3 : 1 ratio. Which halogen is present, and what is the molecular formula?

4. An ester $C_4H_8O_2$ has its base peak at m/z 43, a CH_3CO^+ ion. Is it ethyl ethanoate or methyl propanoate?

5. Which IR evidence shows a sample is propanal and not propan-1-ol?

Fix the mistake

6. Correct this statement: "The tallest peak in the mass spectrum is the molecular ion, so M = 43."

7. Correct this statement: "Propan-2-ol has three carbons, so its ^{13}C NMR spectrum has three peaks."

8. Correct this statement: "There is a dip at 3000 cm^{-1}, so the compound has an O–H group."

9. Correct this statement: "A C=O dip at 1715 cm^{-1} means it is a ketone."

Answer key (for parents and tutors)

1. A C_3H_8O alcohol has a broad IR dip at 3350 cm^{-1} and two peaks in its ^{13}C NMR spectrum. Name it.
   Two peaks means two carbon environments, so it is propan-2-ol, $CH_3CH(OH)CH_3$ (propan-1-ol has three).
2. How many peaks does pentan-3-one, $CH_3CH_2COCH_2CH_3$, give in its ^{13}C NMR spectrum?
   The molecule is symmetrical about the C=O: the two CH_3 are equivalent and the two CH_2 are equivalent, so 3 peaks (CH_3, CH_2 and C=O).
3. A haloalkane has molecular ion peaks at m/z 78 and 80 in a 3 : 1 ratio. Which halogen is present, and what is the molecular formula?
   Two peaks 2 apart in a 3 : 1 ratio show chlorine; 78 − 35 = 43 = C_3H_7, so C_3H_7Cl.
4. An ester $C_4H_8O_2$ has its base peak at m/z 43, a CH_3CO^+ ion. Is it ethyl ethanoate or methyl propanoate?
   Ethyl ethanoate, $CH_3COOCH_2CH_3$, which breaks to CH_3CO^+ (m/z 43); methyl propanoate would give $CH_3CH_2CO^+$ at m/z 57.
5. Which IR evidence shows a sample is propanal and not propan-1-ol?
   A strong sharp C=O dip near 1730 cm^{-1} and no broad O–H dip at 3200 to 3550 cm^{-1}.
6. Correct this statement: "The tallest peak in the mass spectrum is the molecular ion, so M = 43."
   The tallest peak is the base peak, the most common fragment; the molecular ion is the last big peak on the right.
7. Correct this statement: "Propan-2-ol has three carbons, so its ^{13}C NMR spectrum has three peaks."
   The two CH_3 groups are equivalent, so there are two carbon environments and two peaks.
8. Correct this statement: "There is a dip at 3000 cm^{-1}, so the compound has an O–H group."
   C–H dips sit at 2850 to 3000 cm^{-1} in almost every compound; an alcohol O–H is a broad dip at 3200 to 3550 cm^{-1}.
9. Correct this statement: "A C=O dip at 1715 cm^{-1} means it is a ketone."
   Aldehydes, acids, esters and amides all have C=O too; check for O–H or N–H in IR and for the C=O shift in the ^{13}C spectrum.