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ANSWER BOOK

Putting the analysis together: structure from spectra

Organic synthesis · Unit C22

AQA 3.3.15 · OCR A 4.2.4, 6.3.2

11 questions · 33 marks

NAVY EDITION

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SECTION A · Short, 1 to 2 marks

A1 PAT-Q17

B1 exhaled breath is saturated with water vapour, whose O–H bonds absorb strongly across 3200–3600 cm^{-1}, so a reading there would measure the water as well as the ethanol. **B1** near 2950 cm^{-1} the absorption is by the C–H bonds of ethanol, which the other gases in breath do not have, so the absorbance rises with the ethanol concentration alone. [2]

A2 PAT-Q19

B1 the detector's response per gram differs from one compound to another and from one instrument setting to another, so a peak area is not itself a concentration. **B1** standards of the same compound run under the same conditions give the area produced by a known concentration, so the unknown can be read from the line. [2]

SECTION B · Standard, 3 to 5 marks

B1 PAT-Q12

B1 1,4-dimethylbenzene, carbon-13: 3 peaks, for the two equivalent CH_3 carbons, the two ring carbons bearing methyls and the four equivalent ring CH carbons. **B1** 1,4-dimethylbenzene, proton: 2 peaks, the six methyl hydrogens and the four ring hydrogens, in the ratio 6 : 4. **B1** 1,2-dimethylbenzene, carbon-13: 4 peaks, because the mirror plane between the methyls pairs C1 with C2, C3 with C6 and C4 with C5, plus the CH_3 carbons. **B1** 1,2-dimethylbenzene, proton: 3 environments, CH_3 6H, H3 and H6 2H, H4 and H5 2H; allow 2 peaks if the ring hydrogens are said to overlap. [4]

B2 PAT-Q15

B1 the absorption is a C=O and the 209 ppm peak an aldehyde or ketone carbon; five peaks fit pentan-2-one, whose five carbons are all different. **B1** pentan-3-one is ruled out, because its symmetry gives only three carbon peaks. **B1** pentanal also has five carbon environments and a C=O in the same ranges, so these data do not separate it from pentan-2-one; allow 2-methylbutanal in place of pentanal, since it too has five carbon environments. **B1** the conclusion is not yet justified: proton NMR would decide, with a 3H singlet near 2.1 ppm for pentan-2-one or a 1H peak near 9.8 ppm for pentanal. [4]

B3 PAT-Q3

M1 degree of unsaturation = (2C + 2 + N − H) ÷ 2. **A1** C_4H_7N: (8 + 2 + 1 − 7) ÷ 2 = 2, for example the triple bond of a nitrile. **A1** $C_8H_8O_2$: (16 + 2 − 8) ÷ 2 = 5, which suggests a benzene ring (four) and one C=O. [3]

B4 PAT-Q4

B1 the O–H hydrogen exchanges with deuterium, giving O–D. **B1** deuterium does not absorb in the proton NMR spectrum, so the O–H peak disappears when the spectrum is run again. **B1** hydrogens bonded to carbon do not exchange with D_2O, so the CH_3 and CH_2 peaks stay where they were. [3]

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B5 PAT-Q5

B1 ethoxyethane is symmetrical about its oxygen atom. **B1** so its two CH_2 carbons are equivalent and give one peak, and its two CH_3 carbons are equivalent and give another. **B1** in butan-1-ol each carbon has different neighbours, so there are four environments and four peaks. [3]

B6 PAT-Q8

B1 the formula fixes the numbers of carbons, hydrogens and other atoms that every structure must contain. **B1** it gives the degree of unsaturation, which limits how many rings and double bonds the structure can have. **B1** it allows integration ratios to be scaled to real numbers of hydrogens and the carbon-13 peak count to be compared with the number of carbons. [3]

B7 PAT-Q11

B1 butanal shows a peak at 9 to 10 ppm for the aldehyde hydrogen, which butanone does not. **B1** butanone shows a 3H singlet near 2.1 ppm, a CH_3 next to the C=O with no neighbouring hydrogens. **B1** butanone has three hydrogen environments in the ratio 2 : 3 : 3, butanal four in the ratio 1 : 2 : 2 : 3. [3]

B8 PAT-Q14

B1 both give one peak per environment, and the shift of each peak shows what the atoms are bonded to. **B1** proton NMR also gives an integration ratio of the numbers of hydrogens, while carbon-13 peak heights do not give numbers of carbons. **B1** proton NMR shows splitting by neighbouring hydrogens, which shows how groups are joined; carbon-13 spectra at this level show single lines, but they detect carbons with no hydrogens, such as C=O. [3]

B9 PAT-Q16

B1 absorptions at characteristic wavenumbers show which bonds are present, such as C=O at 1680 to 1750 cm^{-1}. **B1** the width and position of an O–H absorption distinguish an alcohol (3230 to 3550 cm^{-1}) from a carboxylic acid (2500 to 3000 cm^{-1}). **B1** it cannot show where in the molecule a group is, or how many carbons there are; the fingerprint region is matched to a database rather than assigned. [3]

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