CH1012 Tutorial 7 Answers

1. A colourless organic liquid which reacted with sodium metal to give an explosive gas gave the following analytical results: C: 64.80% H: 13.50%
Mass spectrum: m/z 74 Infrared spectrum: 3300 cm^{-1} s,br; 2900 cm^{-1} s

- Provide a reasonable **molecular formula**, **structure** and **IUPAC name** for the compound. [1]
- Explain how you came up with this answer.

%O = 100 - (64.80 + 13.50) = 21.70%

nC	= 64.80 / 12.0	nH	= 13.50/1.0	nO	= 21.70 /16.0
	= 5.40		= 13.50		= 1.3564
relative	= 5.40 / 1.3564		= 13.50/1.3564		= 1.3564 /1.3564
	= 3.98		= 9.95		= 1.00
	≈ 4		≈ 10		≈ 1

Empirical formula: $C_4H_{10}O_1$
Molecular formula: $C_4H_{10}O_1$ ⇐ (12.0 x 4) + (10 x 1.0) + (1 x 16.0) = 74 = m/z
Functional groups: from IR hydroxyl group

$CH_3CH_2CH_2CH_2OH$ 1-butanol 

The reaction of this alcohol with Na metal would generate sodium butoxide and hydrogen gas.

2. Explain how you would **purify** a well characterised organic liquid that had been contaminated with an organic solid which had completely dissolved in it.
How would you verify the purity of the purified material?

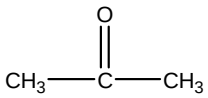
The liquid would be <u>fractionally distilled</u> with the organic solid remaining in the distillation flask (if it had a higher b.p. than the liquid) and the organic liquid being collected in a fraction where the b.p. remained constant. This may have to be repeated several times. To verify the purity of the liquid the b.p. would be compared with the reported value for the organic liquid. Spectroscopy could also be used to check the presence of minor impurities methods such as IR and NMR being most appropriate.

3. Explain how compounds in the following pairs could be **distinguished** on the basis of their IR and NMR spectra (^1H & ^{13}C).

(i) IR: a) ν(OH) 3500 cm^{-1}
b) ν(CO) 1715 cm^{-1}

1H NMR: a) **triplet 2H 4.05**, multiplet 2H 3.10, triplet 3H 1.50, **singlet 5.05** this signal would be removed upon D_2O exchange
b) **singlet 3H 2.01**

$CH_3CH_2CH_2$—OH

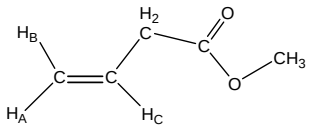


13C NMR: a) CH_2 at 80 ppm (bound to O)
b) C=O at 200 ppm

[1] Atomic masses: C 12.0 H 1.0 O 16.0
IR table see over page

4. Given the following information (formula, IR, NMR) deduce a **structure** for the following organic compound. Detail how you came up with the structure you have chosen.

Molecular formula: $C_5H_8O_2$

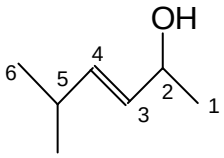


UV: λ l90 nm, ε 1800 C=C
IR(KBr): 2950 (m), 1742 (s), 1625 (s), cm^{-1} 1625 C=C, 1742 C=O ester, 2950 C-H

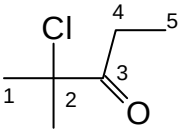
^{1}H NMR ($CDCl_3$): 5.50 (dd, 1H, $=CH_A$), 5.05 (dd, 1H, $=CH_B$), 4.02 (m, 1H, $=CH_C$), 2.51 (d, 2H, $=C-CH_2$), 3.52 (s, 3H, $O-CH_3$) ppm

13C NMR: 167.0 (C=O), 135.0(=CH), 124.5(=CH), 62.0 (O-CH3), 18.2 (CH2)

5. Provide **IUPAC names** for the following molecules:

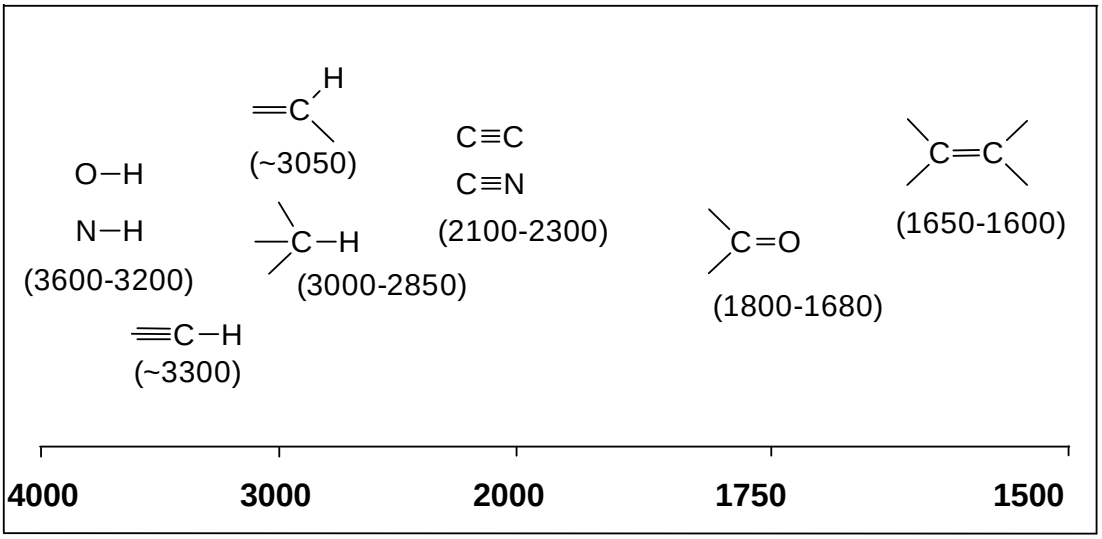


5-methyl-3-hexen-2-ol



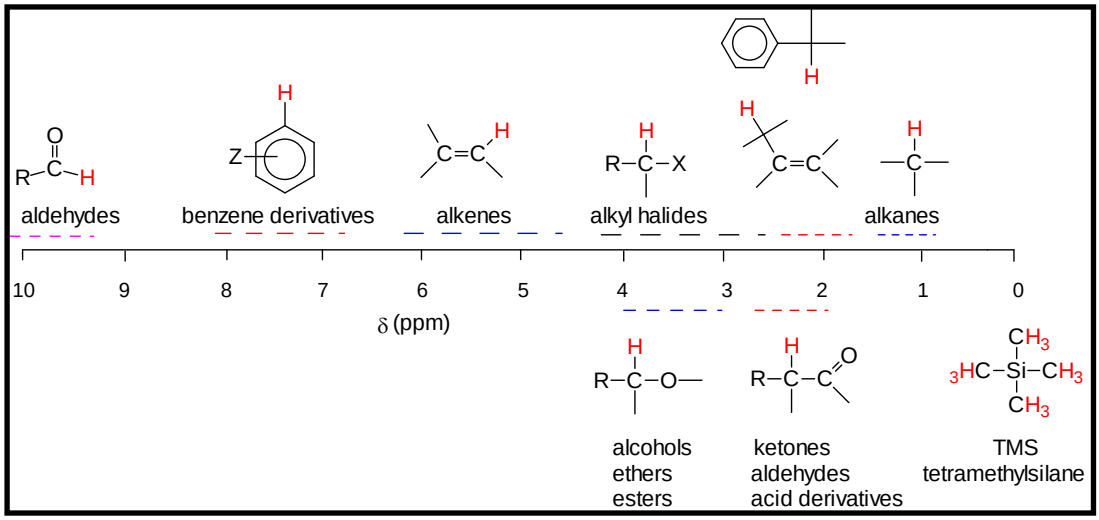
2-chloro-2-methyl-3-pentanone

Chart 1. Typical Infrared frequencies of common functional groups



Wavenumber (cm^{-1}) = 1 / λ (in cm)

Approximate ^{1}H shifts of protons bound to C in some typical organic compounds



Approximate ^{13}C shifts for groups in some typical organic compounds