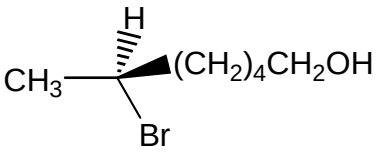
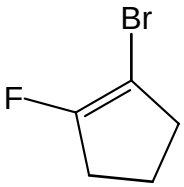
CH1012 Tutorial 7 Answers

1. Provide **IUPAC names** for the following compounds:



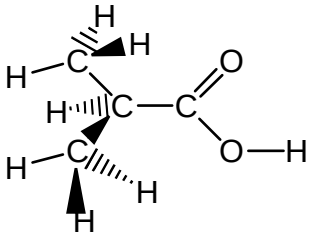


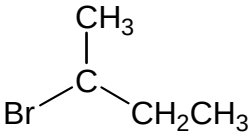
(*S*)-6-bromo-1-heptanol

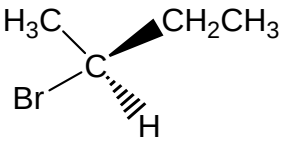
Z-1-bromo-2-fluoro-1-cyclopentene

2. Draw **3D molecular structures** corresponding to the following systematic names:

(a) 2-methylpropanoic acid
(b) (*S*)-2-bromobutane







3. A white crystalline substance gave the following microanalytical results:

C: 68.82 % H: 4.95 %

Infrared spectrum: 3200, 1705 and 1600 cm^{-1}. Mass spectrum: molecular ion m/z 122. The addition of a small quantity of the compound to a solution of Tollen's reagent in ethanol produced no observable change.

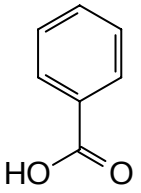
• Give a reasonable **molecular formula**, **skeletal structure** and **IUPAC name** for the compound.
• Explain how you came up with this answer.

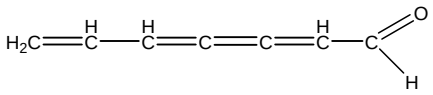
• If the sample became contaminated with a yellow decomposition
• product how would you remove this and then verify the purity of the compound?

	C: 68.82 %	H: 4.95 %	
(100 - 68.82 + 4.95) ⇒			O: 26.23%
÷	12.01;	1.008;	16.00
⇒	5.730	4.911	1.639
÷ 1.639	3.50	3.00	1
x 2	7	6	2

Empirical formula C7H6O2
Molecular formula C7H6O2 (7 x 12) + (6x1) + (2x16) = 122 = m/z
IR information: 3200 cm^{-1} OH 1705 cm-1 carboxylic acid, 1600 cm^{-1} C=C

Reaction information the CO group is not part of an aldehyde functional group as this would have reacted with Tollens reagent to deposit a silver mirror.



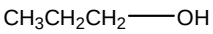


Benzoic acid

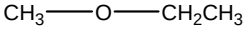
The contaminant is coloured which suggests that it could be removed quite easily by preparative thin layer chromotography. A small amount of the material would be placed on the base of TLC plates and then an appropriate solvent would be used to elute the product and contaminant at different rates.
This would be verified using a UV light to illuminate the benzoic acid. If the band on the plate appeared pure then the benzoic acid would be collected by stripping of the chromographic support with a solvent and then recrystallizing. The recrystallized material would be dried and then a melting point taken - the value would be compared with the literature result to verify the purity of the substance - it should be within +/- 2^{o}C.

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

(i)



(a)



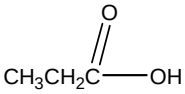
(b)

IR: a) ν(OH) 3500 cm^{-1}
b) –

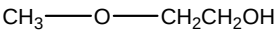
1H NMR: a) triplet, 3H, 1.55; **multiplet, 2H, 1.50**; **triplet, 2H, 3.70;**
singlet, 1H, 5.05 this signal would be removed upon D_2O exchange
b) **singlet, 3H, 3.70; quartet, 2H, 3.70;** triplet, 3H, 1.50;

13C NMR: a) 2 signals at around 30 C-sp^3, 1 signal at around 70 ppm O-C-sp^3
b) 1 signal at around 30 C-sp^3, 2 signals at around 70 ppm O-C-sp^3

(ii)



(a)



(b)

IR: a) ν(OH) 3500 cm^{-1}, **ν(CO) 1700 cm^{-1}**
b) ν(OH) 3500 cm^{-1}

1H NMR: a) **triplet, 3H, 1.50; quartet, 2H, 2.50;**
singlet, 1H, 5.05 this signal would be removed upon D_2O exchange
b) **singlet, 3H, 3.60; triplet, 2H, 3.70; triplet, 2H, 3.50;**
singlet, 1H, 5.05 this signal would be removed upon D_2O exchange

13C NMR: a) 1 signal at around 30 C-sp^3, 1 signal at around 50 ppm (OC)-*C*-sp^3, 1 signal 170 C=O
b) 3 signals at around 70 ppm O-C-sp^3

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

(i) Molecular formula: $C_6H_{12}O_2$

IR: 2900 (CH), 1738 (C=O ester)

^{1}H NMR ($CDCl_3$): δ 4.13 (q, 2H), 2.51 (septet, 1H), 1.26 (t, 3H), 1.18 (d, 6H)

Group OCH2 (C=O)CH CH3 2 x CH3

suggests ester

Adjacent CH3 2 CH3 CH2 CH

^{13}C NMR ($CDCl_3$): δ 170.2, 60.2, 34.0, 19.0, 14.3

C=O sp3-C-O C-sp3 C-sp3 C-sp3

suggests ester

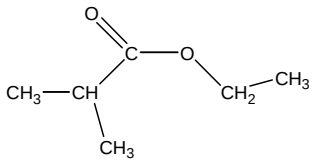
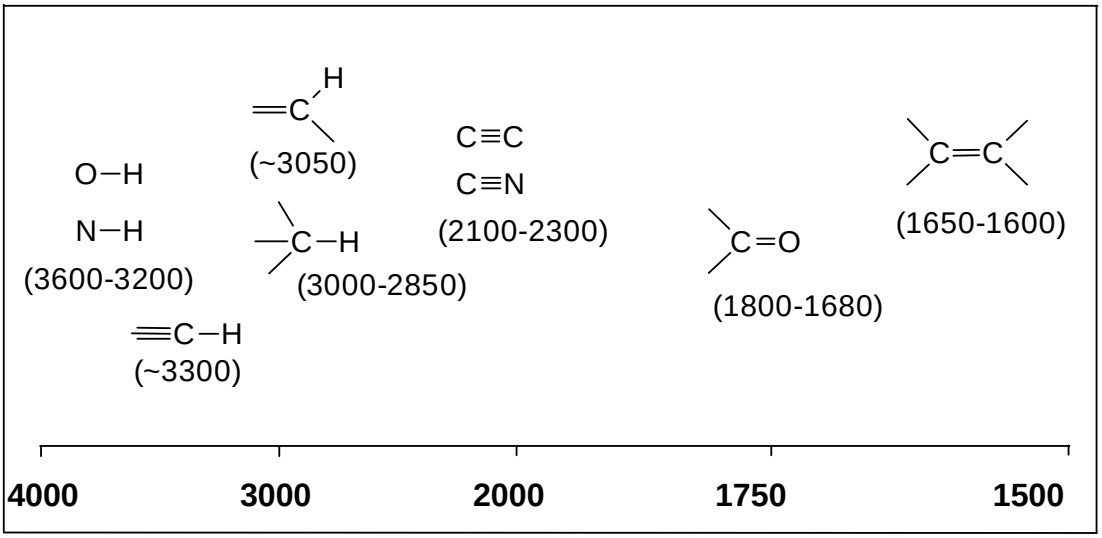
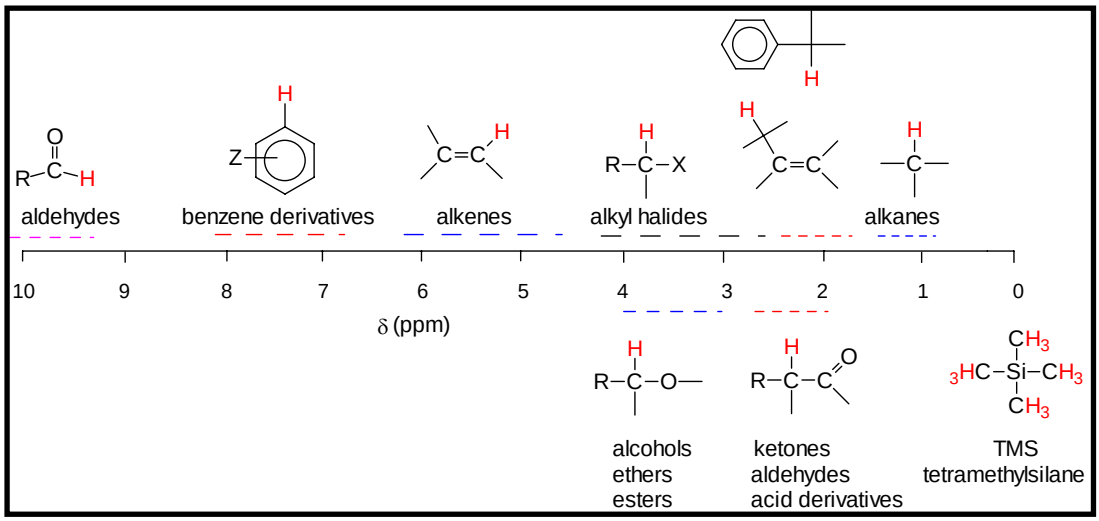


Chart 1. Typical Infrared frequencies of common functional groups



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