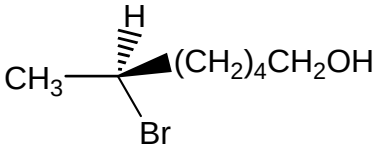
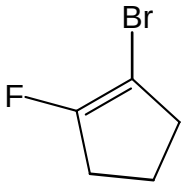
CH1012 Tutorial 7

Name:

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



(a)



(b)

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 %

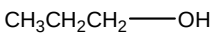
Infrared spectrum: 3200, 1705 and 1600 cm^{-1}. Mass spectrum: molecular ion m/z 122.
The addition of a small quantity of the compound to a solution of Tollen's reagent in ethanol produced no observable change.

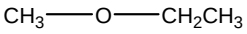
• Give a reasonable **molecular formula**, **skeletal structure** and **IUPAC name** for the compound.
• Explain how you came up with this answer.

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

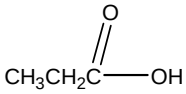
4. Explain how compounds in the following pairs could be distinguished on the basis of their IR and NMR spectra (^{1}H & ^{13}C).

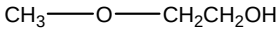
(i)





(i)





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.

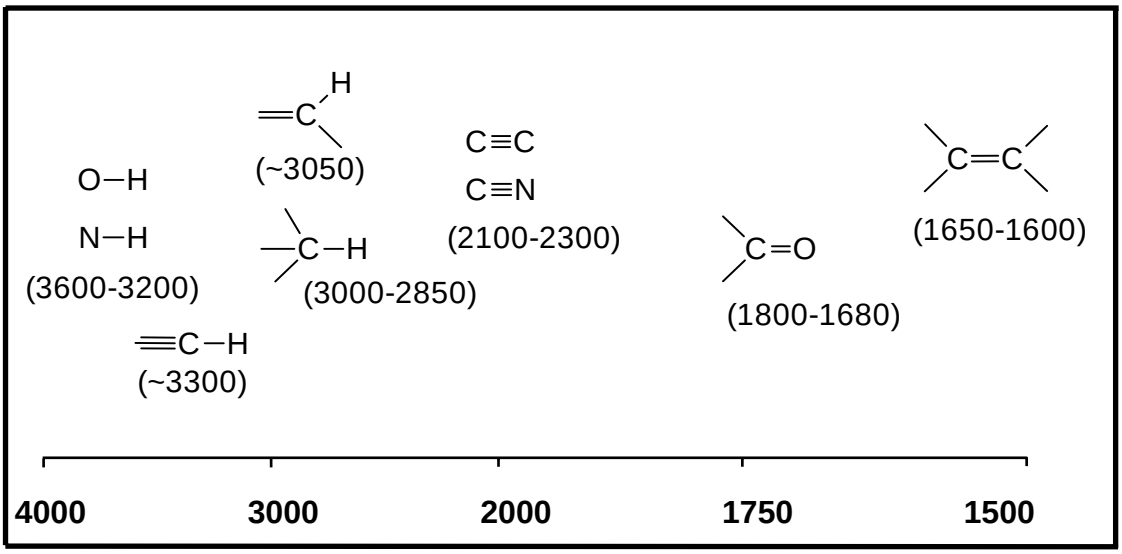
Molecular formula: $C_6H_{12}O_2$

IR(KBr): 2900 (m), 1738 (s) cm^{-1}

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

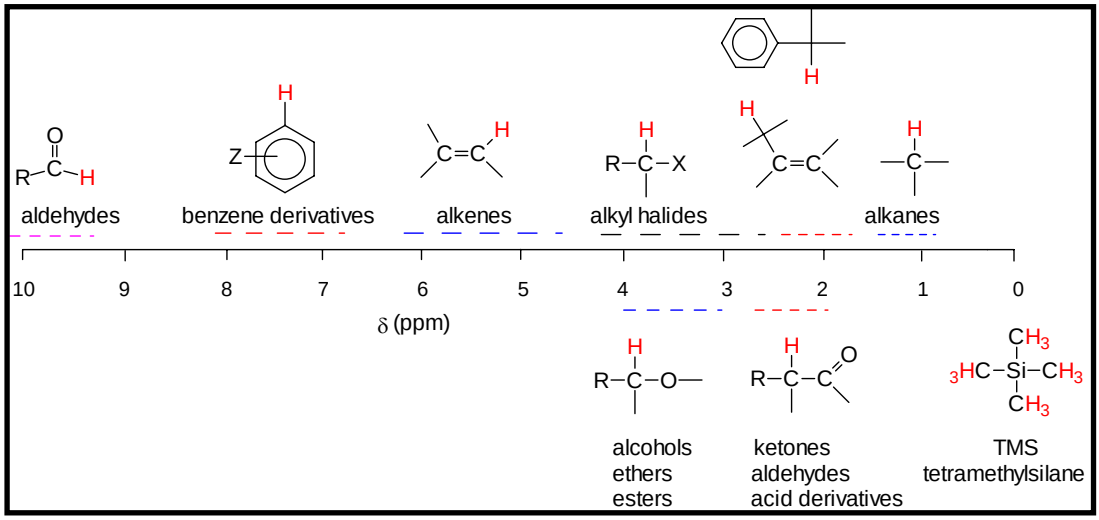
^{13}C NMR ($CDCl_3$): δ 170.2, 60.2, 34.0, 19.0, 14.3 ppm

Chart 1. Typical Infrared (IR) frequencies of common functional groups



Carbonyl Absorptions ν (cm^{-1}) **Acid chlorides** ~ 1790**; Esters** ~ 1740**;**
Aldehydes ~ 1720**; Ketones** ~ 1710**; Acids** ~ 1700

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



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