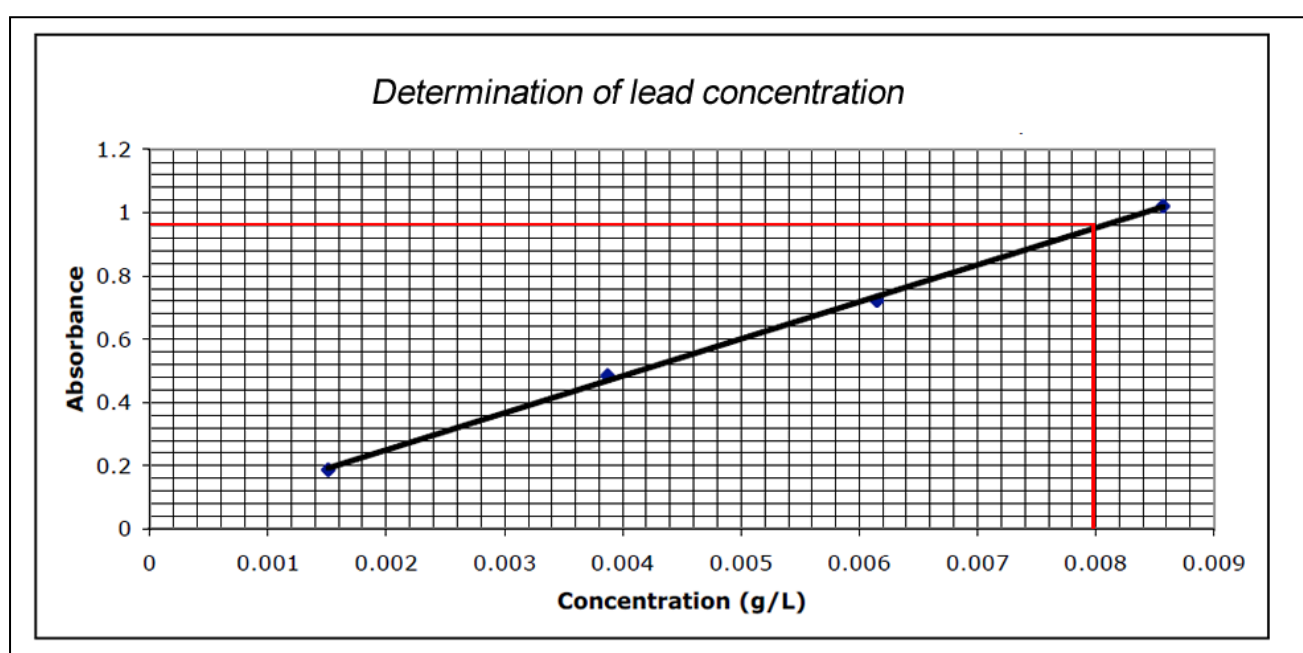


Revision Unit 3 and 4 worksheet 1

- 1) A sample of contaminated water was analysed for its lead content. Using a spectroscopic technique the absorbance of 4 solutions of accurately known lead concentration was measured. The results are shown in the table below.

Absorbance	Concentration (g/L)
0.200	0.00125
0.440	0.00383
0.660	0.00618
1.050	0.00860



- a) Draw a calibration curve using the set of axis shown above.
- b) What technique is best suited for this analysis? Explain
Atomic absorption spectroscopy.
- c) Describe the key components of this technique. What makes this technique so accurate for the analysis of lead concentrations?
- d) A 20.0 mL sample of the original water was placed in a 250 mL volumetric flask and made up to the mark with distilled water. A 20.0 mL sample was then taken from the volumetric flask and placed in a clean beaker. A 2.00 mL sample was then taken from the beaker and diluted by the addition of 8.00 mL of water. This 10.0 mL sample was then analysed and found to have an absorbance reading of 0.880. Find the concentration of the original sample of water in mol/litre.

Step 1 According to the calibration curve an absorbance of 0.880 equates to a concentration of 0.00800 g/L.

Step 2 Find the amount, in grams, of lead in the 10.0 mL sample analysed

$$\text{mass} = C \times V = 0.00800 \text{ g/L} \times 0.01 = 8.00 \times 10^{-5}$$

Step 3 find the mass of lead in the 20.0 mL sample placed in the beaker

$$\text{mass} = 8.00 \times 10^{-5} \times 20.0/2.00 = 8.00 \times 10^{-4}$$

Step 4 find the total mass of lead in grams in the volumetric flask and hence from the 20.0mL sample

$$\text{mass} = 8.00 \times 10^{-4} \times 250.0/20.0 = 1.00 \times 10^{-2}$$

Step 5 find the mol of lead in the 20.0 mL sample

$$n_{\text{Pb}} = 0.001 / 207.2 = 4.83 \times 10^{-5}$$

Step 6 find the molarity of lead in the original 20.0 mL sample

$$M = n/V = 4.83 \times 10^{-5} / 0.02 = 2.42 \times 10^{-3} \text{ M}$$

e) What is the concentration of lead in the sample in ppm?

Step 1 find the mass of lead in mg present in the original sample of 20.0 mL

$$\Rightarrow 1.00 \times 10^{-2} \text{ g} = 10.0 \text{ mg}$$

Step 2 convert concentration to mg/L

$$\Rightarrow 10.0/0.200 = 50.0 \text{ ppm}$$

f) World Health Organisation studies have linked lead concentrations of 50 µg/l with neurological damage.

i. What is the concentration of 50 µg/l of lead in ppm?

$$50 \mu\text{g/l} = 0.05 \text{ mg/L} = 0.05 \text{ ppm}$$

ii. What volume of pure water, in litres, must be added to 2.00 litres of the original water sample so that the final concentration of lead is 0.005 ppm?

$$C_1 V_1 = C_2 V_2$$

$$C_1 = 50.0 \text{ mg/L} = 0.0500 \text{ ppm}$$

$$V_1 = 2.00 \text{ L}$$

$$C_2 = 0.00500 \text{ ppm}$$

$$V_2 = ?$$

$$\Rightarrow V_2 = C_1 V_1 / C_2 = 0.0500 \times 0.02 / 0.00500 = 20.0 \text{ litres}$$

Hence 18.0 litres must be added.

2) An unknown compound "X" was analysed and found to contain 64.9 % C, 21.6% O and 13.5% H by mass. The mass spectrum of this compound is shown on the right. Using the information provided

a) Calculate the empirical formula of compound "X"

Assume 100 grams of the product.

Hence

64.9 g of C, 21.6g of O, 13.5g of H

Step 1 Convert to mol ratio.

$$\Rightarrow \underline{64.9} \text{ C}, \underline{21.6} \text{ O}, \underline{13.5} \text{ H}$$

$$12.0 \quad 16.0 \quad 1.0$$

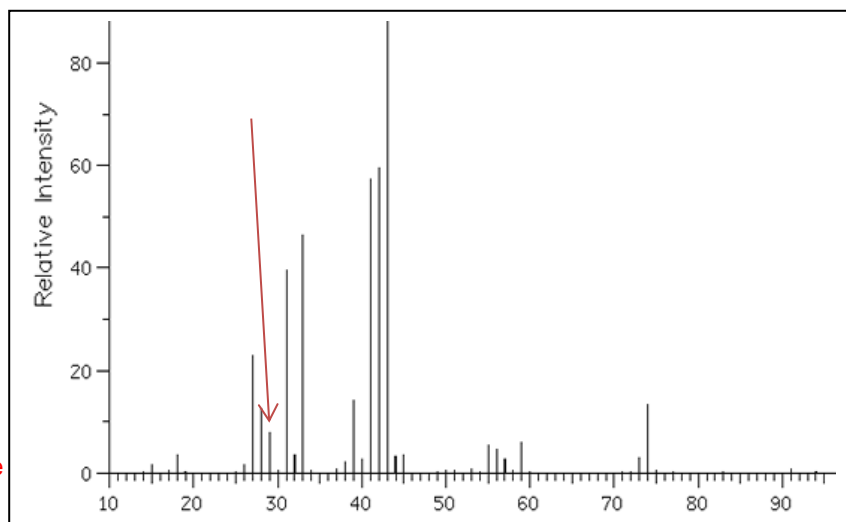
$$\Rightarrow 5.41 \text{ C} : 1.35 \text{ O} : 13.5 \text{ H}$$

Step 2 Obtain the simplest ratio

$$\Rightarrow 5.41/1.35 : 1.35/1.35 : 13.5/1.35$$

$$\Rightarrow 4 \text{ C} : 1 \text{ O} : 10 \text{ H}$$

Step 3 Since all numbers are whole



b) Give the molecular formula of compound "X".

From the MS we can find that the parent ion has a molecular mass of 74

Hence we can work out the ratio

empirical mass : Formula mass

=> 74 : 74 = 1 : 1

This tells us that the empirical formula is the same as the molecular formula

$C_4H_{10}O$

c) Consider the mass spectrum of compound "X", given above.

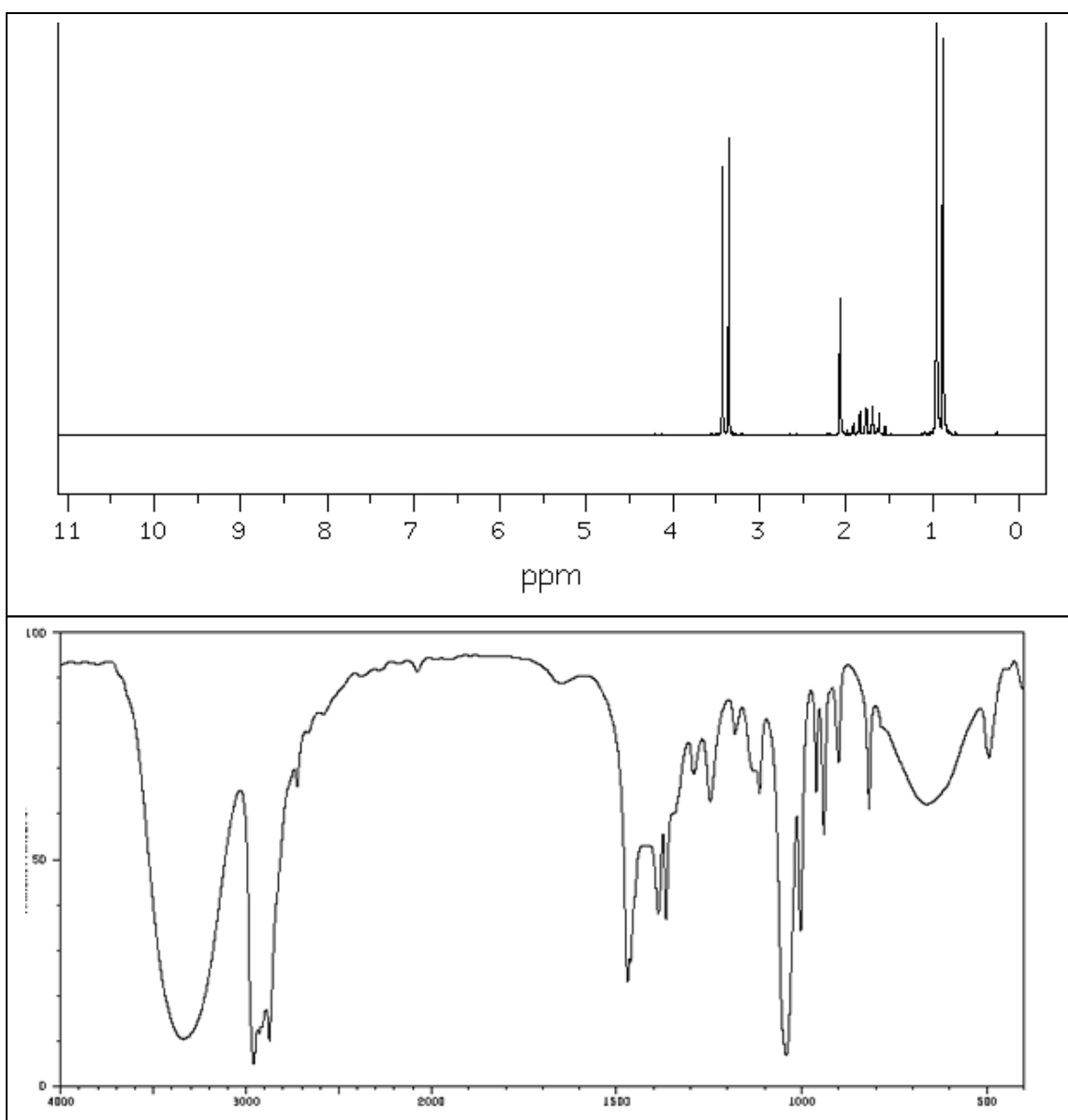
i. What are the units of the X-axis

Mass of fragment /charge of fragment

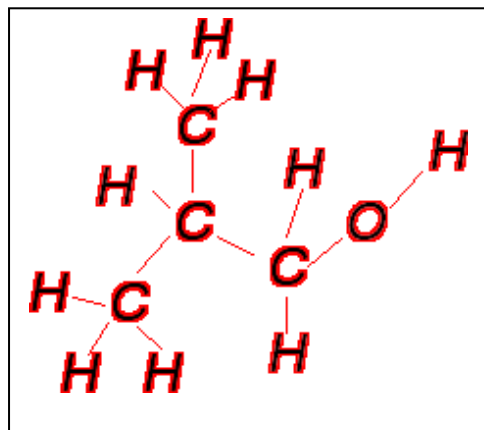
ii. Explain how the peak at 29, on the axis, indicated by the arrow was formed.

The Fragment $CH_3CH_2^+$ is represented by the peak at m/z 29.

d) Below are the H^1 NMR and IR spectra of compound "X".



- i. Identify the compound giving its IUPAC name.
2-methylpropan-1-ol or 2-methyl-1-propanol
- ii. What information about the compound is revealed by the IR spectrum?
The broad absorption trough at wavelength 3300-3400 indicates an alcohol -OH and a C-O bond at a wavelength around 1100.
- iii. Give the structural formula of the compound



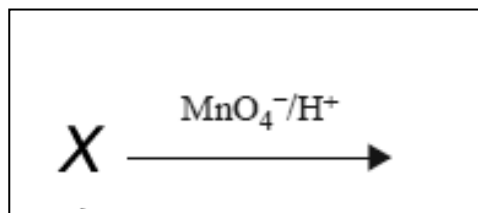
- e) What is the IUPAC name of the product of the reaction pictured on the right?

2-methylpropanoic acid

Since X is 2-methylpropan-1-ol an oxidation reaction will yield propanoic acid

The methyl group comes off the second carbon.

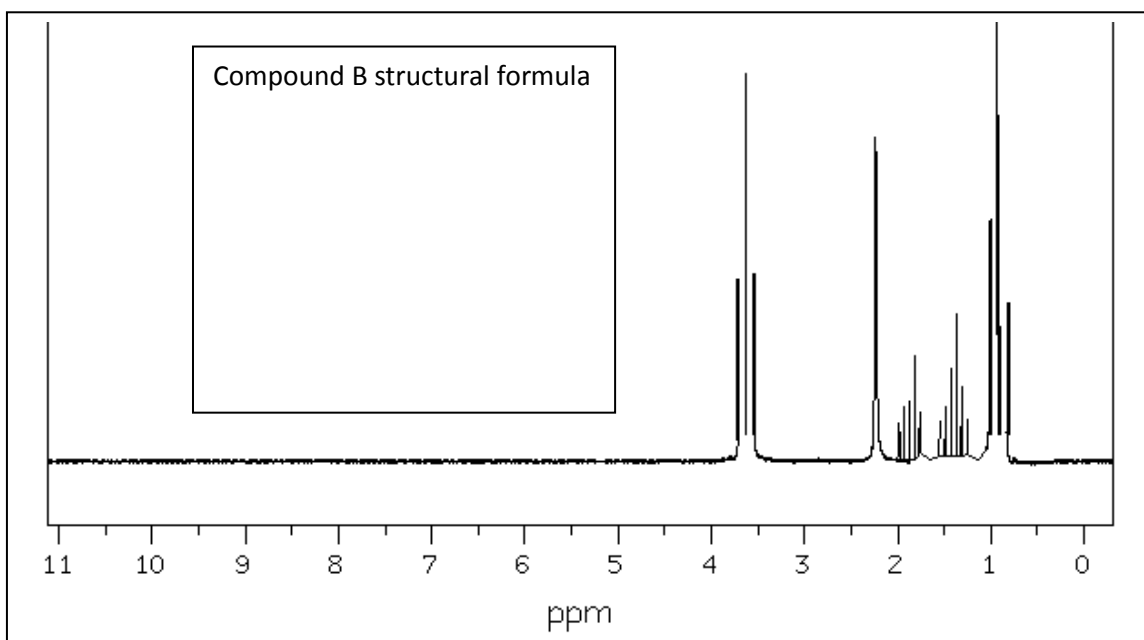
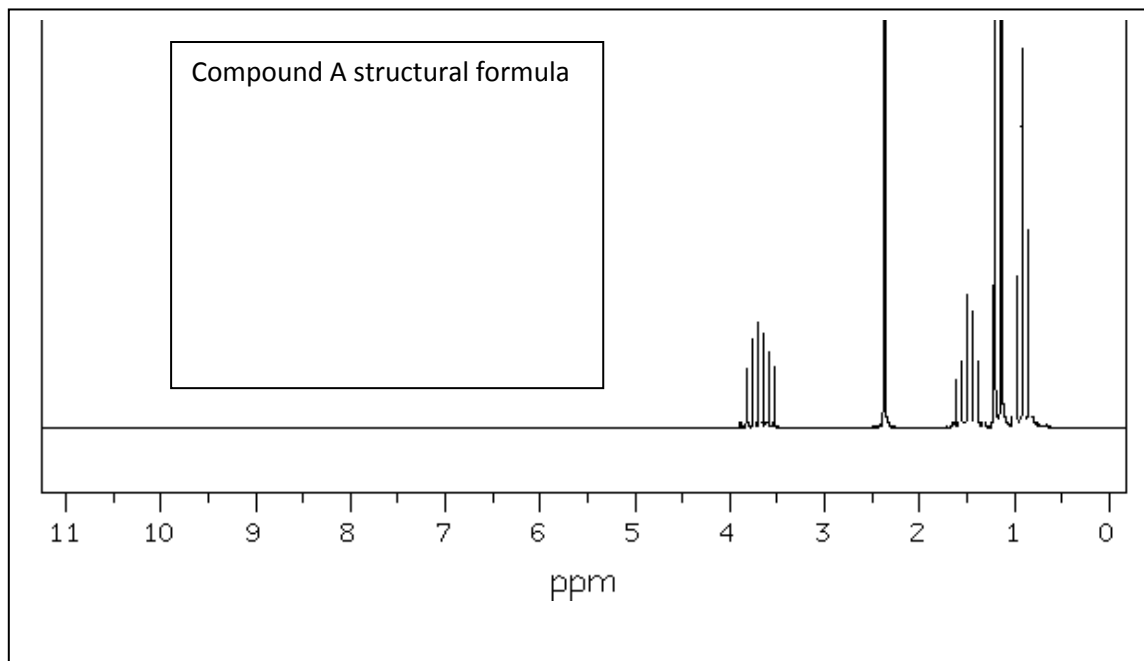
Numbering of carbons starts from the functional group. Only primary alcohols can be oxidised to form carboxylic acids.



f) Below are two compounds with the same molecular formula as the unknown compound above. Give the IUPAC name of each. They are isomers of the compound above and hence have the same molecular formula but different structural formula.

A. _____ **butan-2-ol** _____

B. _____ **butan-1-ol** _____



g) There are four isomers with the molecular formula of compound "X". Three are mentioned here, in the question above.

i. What is the IUPAC name of the fourth isomer?

2-methylpropan-2-ol

ii. Explain how the H^1 NMR spectra of compound "B" above and this fourth compound differ. The fourth isomer has only two singlets in the H^1 NMR spectrum. It only has two hydrogen environments.

