



HIGH RESOLUTION MASS SPECTROMETRY

- 1) A compound is found to have an accurate relative formula mass of 46.0417. It is thought to be either $\text{CH}_3\text{CH}_2\text{OH}$ or $\text{H}_2\text{NCH}_2\text{NH}_2$. Calculate the M_r of each compound to 4 decimal places to work out which one it is.

$\text{CH}_3\text{CH}_2\text{OH}$ **46.0417**

$\text{H}_2\text{NCH}_2\text{NH}_2$ **46.0530**

Molecular formula = **$\text{C}_2\text{H}_6\text{O}$**

- 2) Analysis of an organic compound showed that its relative formula mass is 102. High resolution mass spectroscopy showed it to be 102.0678.

- a) Which of the following three molecular formulas could the compound have? Calculate the M_r of each compound to 4 decimal places to do this.

$\text{C}_5\text{H}_{14}\text{N}_2$ **102.1154**

$\text{C}_5\text{H}_{10}\text{O}_2$ **102.0678**

$\text{C}_3\text{H}_6\text{N}_2\text{O}_2$ **102.0428**

Molecular formula = **$\text{C}_5\text{H}_{10}\text{O}_2$**

- b) Draw and name two molecules that this could be.

$\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-COOH}$ *pentanoic acid*

$\text{CH}_3\text{-CH}(\text{CH}_3)\text{-CH}_2\text{-COOH}$ *3-methylbutanoic acid*

- 3) Calculate the accurate mass of the two molecular ion peaks in the high resolution mass spectrum of chloroethane.

Peak 1 **64.0079**

Peak 2 **66.0049**

- 4) How could high resolution mass spectroscopy be used to distinguish propane and ethenol?

M_r of propane $\text{CH}_3\text{-CH}_2\text{-CH}_3 = 44.0624$

M_r of ethenol $\text{CH}_2\text{=CH-OH} = 44.0261$

Measure the M_r to 4 dp and see if it is 44.0624 or 44.0261