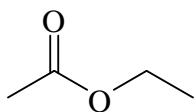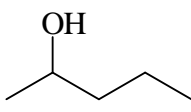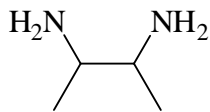**Marks
3**

- Suppose a molecule has been isolated from a natural source. When a sample of the molecule is analysed by low resolution mass spectrometry, it shows a molecular ion peak that implies the molecule has a molecular weight of 88. You determine that the molecule might be one of the following three possibilities, all of which have a molecular weight of 88.

A   **B**   **C**

Further data are acquired for the compound as follows:

- Elemental analysis data: C, 68.13%; H, 13.72% (another element is also present)

- High resolution mass spectrum suggests the molecular weight is actually 88.0888.

Explain how *either* high resolution mass spectrometry *or* the elemental analysis data allows you to distinguish between these three possibilities and hence identify which of **A**, **B** or **C** is in the sample.

Information you may need:

Average atomic masses: C: 12.0107,   H: 1.0079,   O: 15.9994,   N: 14.0067
Exact isotopic masses: ^{12}C: 12.0000, ^{1}H: 1.0078, ^{16}O: 15.9949, ^{14}N: 14.0031

Using the high resolution mass spectra:

A ($C_4H_8O_2$) has MW = 4 × 12.0000 + 8 × 1.0078 + 2 × 15.9949 = 88.0522

B ($C_5H_{12}O$) has MW = 5 × 12.0000 + 12 × 1.0078 + 15.9949 = 88.0885

C ($C_4H_{12}N_2$) has MW = 4 × 12.0000 + 12 × 1.0078 + 2 × 14.0031 = 88.0998

The unknown compound has a high resolution molecular ion peak of 88.0888 which is very close to the expected value for compound B.

Using elemental analysis, the unknown compound has a C:H ratio of

68.13/12.0107 : 13.72/1.0079 = 5.672 : 13.61 ≈ 1 : 2.4

A ($C_4H_8O_2$) has C:H = 4 : 8 = 1 : 2

B ($C_5H_{12}O$) has C:H = 5 : 12 = 1 : 2.4

C ($C_4H_{12}N_2$) has C:H = 4 : 12 = 1 : 3

Therefore the unknown is compound B.