Formulae and Structures Map

Edexcel A Level Chemistry · Topic 18C Formulae and Structures

1 Percentage composition

18C.18

- Divide each % by Ar
- Divide by the smallest
- Gives the **empirical formula**
- Mr gives the molecular formula



2 Combustion analysis

18C.18

- CO_2 gives moles of C
- H_2O: **two H each**
- O by difference in mass
- Then the same ratio

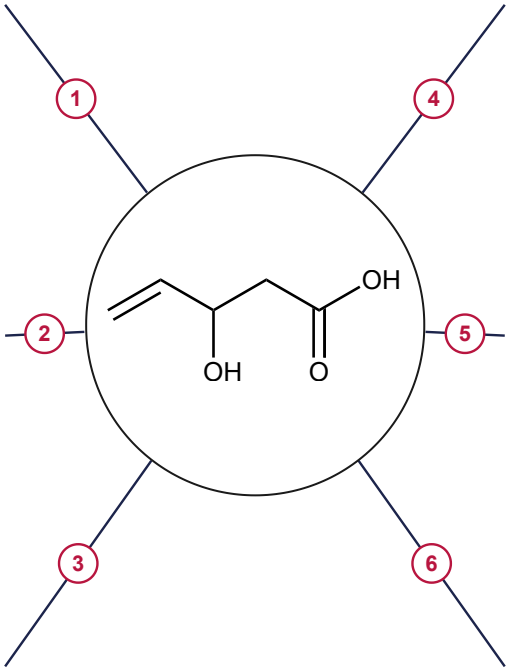


3 Chemical tests

18C.18

- Each test: one group
- Give the **observation**
- Use more than one
- Table below

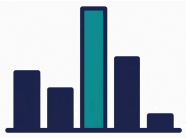




4 Mass spectra

18C.18

- M^+ peak gives Mr
- Loss of 15: CH_3
- Loss of 29: C_2H_5
- m/z 43: CH_3CO^+ or $C_3H_7^+$



5 Infrared spectra

18C.18

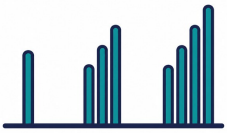
- C=O near 1700 cm^{-1}
- O–H in alcohols, broad
- O–H in acids, very broad
- Use the data sheet



6 NMR spectra

18C.18

- ^{13}C: peaks = environments
- ^1H: area gives H ratio
- ^1H: n + 1 splitting
- δ shows the environment



Tests for functional groups

the reagent and what is seen

Reagent	Seen	Shows
Bromine water	Orange to colourless	C=C
2,4-DNPH	Orange precipitate	C=O
Tollens' reagent	Silver mirror	Aldehyde
Na_2CO_3(aq)	Fizzing, CO_2	COOH
PCl_5	Misty fumes of HCl	OH

Worked examples

From percentages

- C 40.0, H 6.7, O 53.3
- Ratio 1 : 2 : 1; Mr 60
- **$C_2H_4O_2$**

From combustion

- 0.580 g burns to
- 1.32 g CO_2, 0.540 g H_2O
- **C_3H_6O**

From spectra

- Mr 58; C=O in IR
- One ^1H NMR peak
- **Propanone**

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