

Infrared Spectroscopy and Mass Spectrometry

Functional groups, molar mass and fragments

Name _____ Class _____ Date _____

IR AND MS DATA

IR (cm^{-1}): O-H alcohol 3200–3550 broad · O-H acid 2500–3300 very broad · N-H 3300–3500 · C-H 2850–3100 · $\text{C}\equiv\text{N}$ 2250 · C=O 1680–1750 · C=C 1620–1680 · C-O 1000–1300

MS fragments: 15 CH_3^+ · 29 C_2H_5^+ / CHO^+ · 31 CH_2OH^+ · 43 C_3H_7^+ / CH_3CO^+ · 45 COOH^+ · Cl: M : M+2 = 3 : 1 · Br: 1 : 1

Isotopes: ^{79}Br 78.918 (50.69 %) · ^{81}Br 80.916 (49.31 %) · $\lambda = 1/(\text{wavenumber}) \cdot 1 \text{ cm} = 10^4 \mu\text{m}$

Show units in every calculation step.

A. IR spectroscopy

1. (a) What happens to a bond when it absorbs infrared radiation? (b) What is the fingerprint region, and how is it used?

2. Identify the functional group(s) indicated by: (a) broad 3400 cm^{-1} and 1100 cm^{-1} (b) strong 1720 cm^{-1} only (c) very broad 2500–3300 cm^{-1} and 1705 cm^{-1} (d) sharp 2250 cm^{-1}

3. Convert to wavelength in μm : (a) 3300 cm^{-1} (b) 2250 cm^{-1}

4. Explain how IR spectroscopy could distinguish between propan-1-ol, propanal and propanoic acid.

B. Mass spectrometry

5. Butanone, $\text{CH}_3\text{COCH}_2\text{CH}_3$, has peaks at m/z 72, 57, 43 and 29. Identify the molecular ion and the ion responsible for each fragment.

6. A compound shows peaks at m/z 78 and 80 in a 3 : 1 ratio; another shows peaks at 122 and 124 in a 1 : 1 ratio. What halogen does each contain?

7. Use the isotope data to calculate the relative atomic mass of bromine.

C. Challenge

8. An unknown $\text{C}_2\text{H}_4\text{O}_2$ has IR absorptions at $2500\text{--}3300\text{ cm}^{-1}$ (very broad) and 1710 cm^{-1} . Its mass spectrum has peaks at m/z 60, 45, 43 and 15. Identify the compound and explain each piece of evidence.