

# Infrared Spectroscopy and Mass Spectrometry

Answer key with worked solutions

## A. IR spectroscopy

### 1. IR basics.

(a) The bond **vibrates** more strongly (stretches or bends): it absorbs the energy of IR radiation at a wavenumber characteristic of that bond. (b) The region **below about 1500 cm<sup>-1</sup>**: a complex pattern unique to each compound, **compared with a database** of known spectra to confirm an identity.

### 2. Functional groups.

(a) **alcohol** (O-H and C-O) (b) **C=O** with no O-H: a ketone, aldehyde or ester (c) **carboxylic acid** (very broad O-H and C=O) (d) **nitrile**, C≡N

### 3. Wavelengths.

$$\begin{aligned}\text{(a) } \lambda &= \frac{1}{3300 \text{ cm}^{-1}} = 3.030 \times 10^{-4} \text{ cm} \times \frac{10^4 \mu\text{m}}{1 \text{ cm}} = \mathbf{3.03 \mu\text{m}} \\ \text{(b) } \lambda &= \frac{1}{2250 \text{ cm}^{-1}} = 4.444 \times 10^{-4} \text{ cm} = \mathbf{4.44 \mu\text{m}}\end{aligned}$$

### 4. Three C<sub>3</sub> compounds.

**Propan-1-ol**: broad O-H at 3200–3550 cm<sup>-1</sup>, **no C=O**. **Propanal**: strong C=O at about 1730 cm<sup>-1</sup>, **no O-H**. **Propanoic acid**: **both** a very broad O-H (2500–3300 cm<sup>-1</sup>) and a C=O.

## B. Mass spectrometry

### 5. Butanone.

**72**: molecular ion [CH<sub>3</sub>COCH<sub>2</sub>CH<sub>3</sub>]<sup>+</sup> (C<sub>4</sub>H<sub>8</sub>O, 72). **57**: CH<sub>3</sub>CH<sub>2</sub>CO<sup>+</sup> (loss of CH<sub>3</sub>, 72 – 15). **43**: CH<sub>3</sub>CO<sup>+</sup> (loss of C<sub>2</sub>H<sub>5</sub>, 72 – 29). **29**: C<sub>2</sub>H<sub>5</sub><sup>+</sup>.

### 6. Halogens.

3 : 1 for M and M+2: **chlorine** (one Cl atom). 1 : 1: **bromine** (one Br atom).

7. Bromine.

$$A_r = 78.918 \times 0.5069 + 80.916 \times 0.4931$$
$$= \mathbf{79.90}$$

## C. Challenge

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8. The unknown.

**Ethanoic acid**,  $\text{CH}_3\text{COOH}$ . Very broad  $2500\text{--}3300\text{ cm}^{-1}$ : **acid O-H**;  $1710\text{ cm}^{-1}$ : **C=O**. MS: **60** = molecular ion ( $\text{C}_2\text{H}_4\text{O}_2$ , 60 g/mol); **45** =  $\text{COOH}^+$  (loss of  $\text{CH}_3$ ); **43** =  $\text{CH}_3\text{CO}^+$  (loss of OH,  $60 - 17$ ); **15** =  $\text{CH}_3^+$ .