



# ORGANIC ANALYSIS

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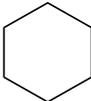


Functional group	Test	Positive result	Negative result
C=C alkene	add a few drops of bromine water	(orange solution →) colourless solution	no change
O-H in primary & secondary alcohol (also works with aldehyde)	warm with acidified potassium dichromate(VI)	(orange solution →) green solution	no change
-CHO aldehyde	warm with Tollens' reagent	(colourless solution →) silver mirror	no change
	warm with Fehling's solution	(blue solution →) orange-red precipitate	no change
-COOH carboxylic acid	add sodium carbonate	bubbles / effervescence	no change
-Cl / -Br / -I halogenoalkane	warm with sodium hydroxide and then add silver nitrate	(colourless solution →) white precipitate (-Cl) cream precipitate (-Br) yellow precipitate (-I)	no change

### TASK 1 – Chemical tests

For each pair of compounds, state reagent(s) that could be used to distinguish the compounds and give the result for each compound.

<b>PAIR 1</b> Compound	$\begin{array}{c} \text{CH}_3 - \text{CH} - \text{CH}_3 \\   \\ \text{OH} \end{array}$	$\begin{array}{c} \text{CH}_3 - \text{C} - \text{CH}_3 \\    \\ \text{O} \end{array}$
Test	warm with acidified potassium dichromate(VI)	
Result	(orange solution →) green solution	no change

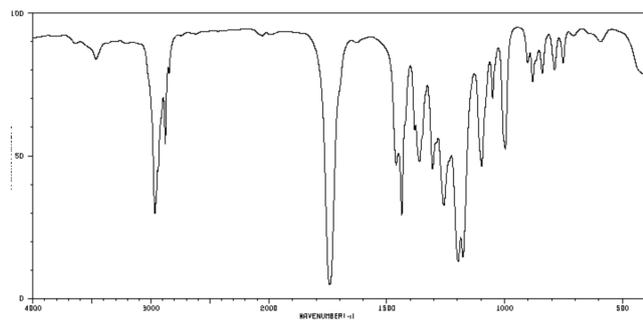
<b>PAIR 2</b> Compound		
Test	add a few drops of bromine water	

Result	<b>no change</b>	<b>(orange solution →) colourless solution</b>
<b>PAIR 3</b> Compound	$\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_3 - \text{C} - \text{CH}_2 - \text{CH}_3 \\   \\ \text{OH} \end{array}$	$\begin{array}{c} \text{CH}_3 - \text{CH} - \text{CH}_2 - \text{CH}_3 \\   \\ \text{OH} \end{array}$
Test	<b>warm with acidified potassium dichromate(VI)</b>	
Result	<b>no change</b>	<b>(orange solution →) green solution</b>
<b>PAIR 4</b> Compound	$\begin{array}{c} \text{O} \\    \\ \text{CH}_3 - \text{C} - \text{CH}_2 - \text{CH}_3 \end{array}$	$\begin{array}{c} \text{O} \\    \\ \text{CH}_3 - \text{CH}_2 - \text{CH}_2 - \text{C} - \text{H} \end{array}$
Test	<b>warm with Tollens' reagent OR warm with Fehling's solution</b>	
Result	<b>no change</b>	<b>(colourless solution →) silver mirror OR (blue solution →) orange-red precipitate</b>
<b>PAIR 5</b> Compound	$\begin{array}{c} \text{O} \\    \\ \text{CH}_3 - \text{C} - \text{CH}_2 - \text{CH}_3 \end{array}$	$\begin{array}{c} \text{O} \\    \\ \text{CH}_3 - \text{CH}_2 - \text{C} - \text{OH} \end{array}$
Test	<b>add sodium carbonate</b>	
Result	<b>no change</b>	<b>bubbles / effervescence</b>
<b>PAIR 6</b> Compound	$\begin{array}{c} \text{O} \\    \\ \text{CH}_3 - \text{C} - \text{CH}_3 \end{array}$	$\text{CH}_3 - \text{CH} = \text{CH} - \text{CH}_3$
Test	<b>add a few drops of bromine water</b>	
Result	<b>no change</b>	<b>(orange solution →) colourless solution</b>

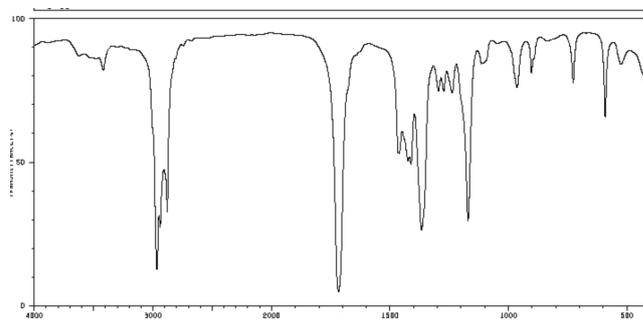
## TASK 2 – IR Problems A

Which of these compounds contain a C=O bond?

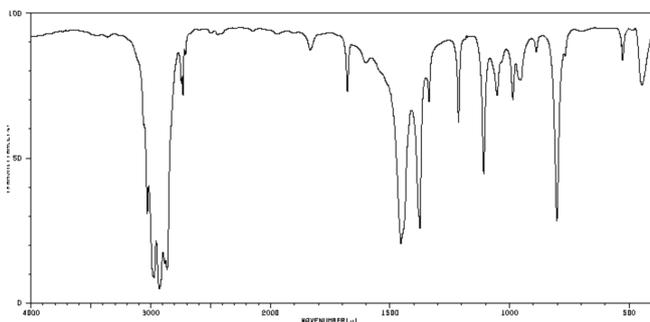
A1 ✓



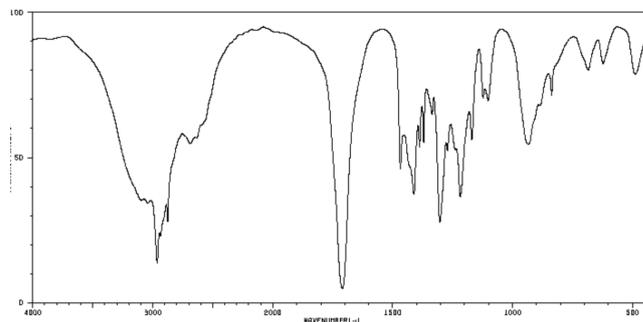
A2 ✓



A3 ✗

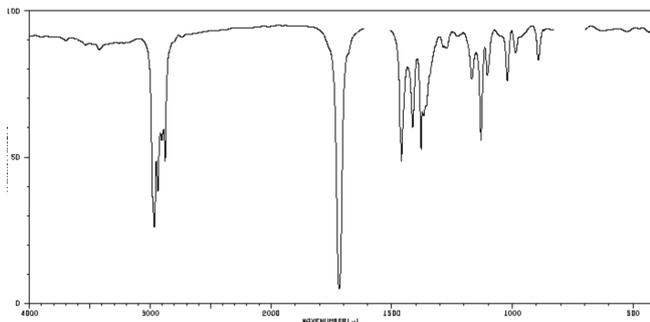


A4 ✓

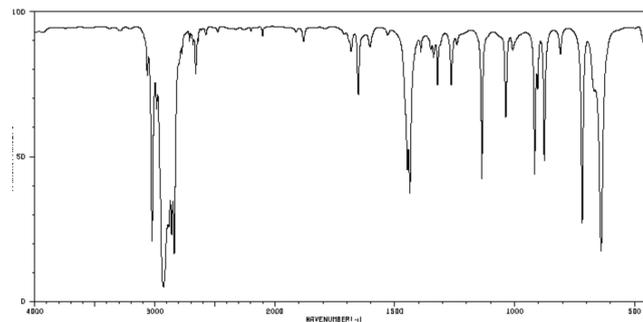


Which of these compounds contain a C=C bond?

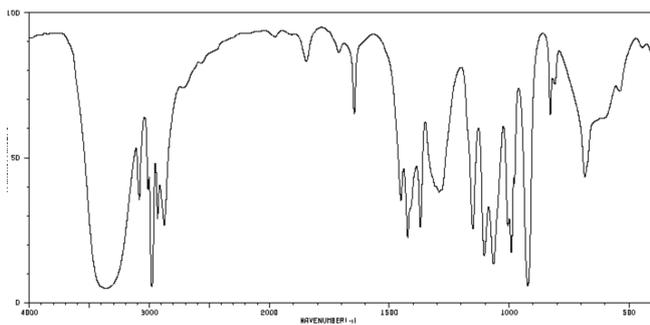
B1 ✗



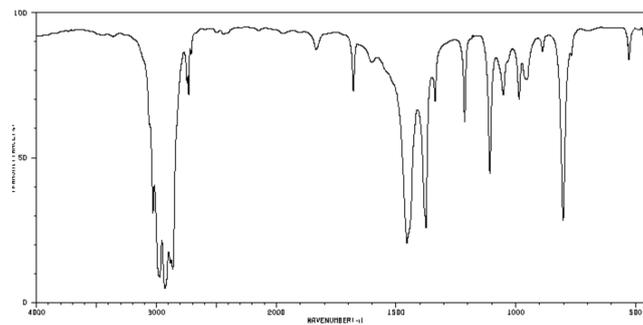
B2 ✓



B3 ✓

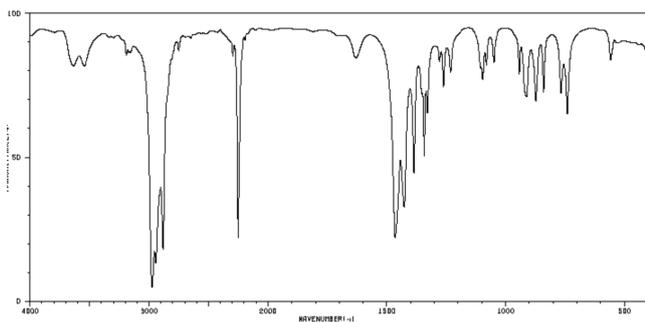


B4 ✓

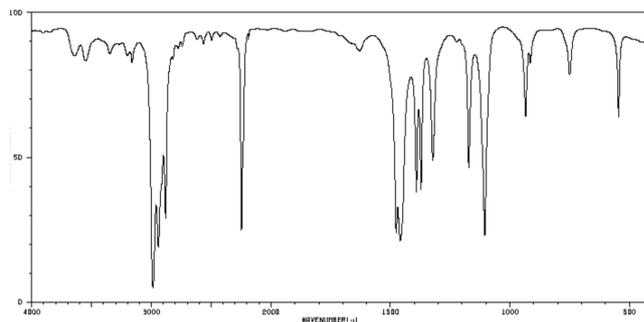


Which of these compounds contain a C≡N bond?

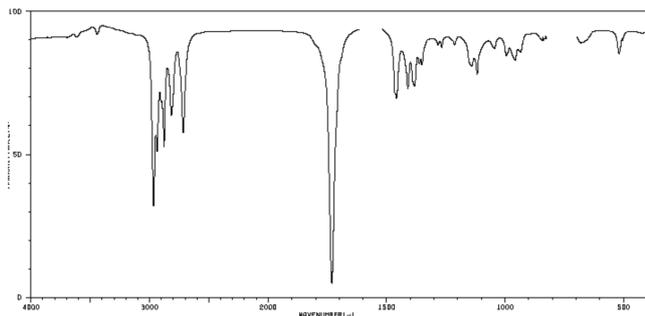
C1 ✓



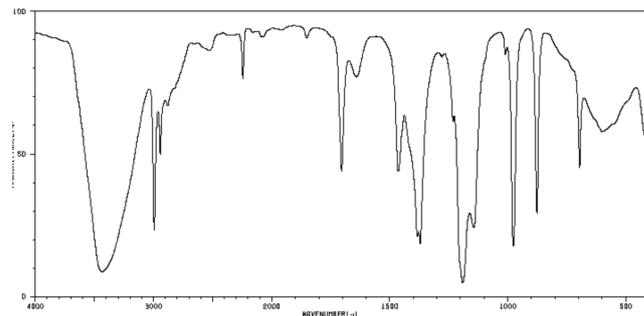
C2 ✓



C3 ✗

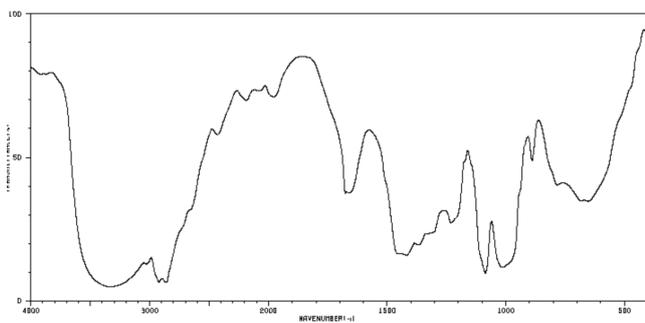


C4 ✓

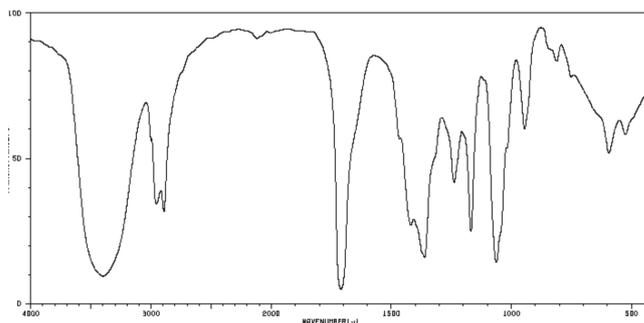


Which of these compounds contain an O-H (acid) bond?

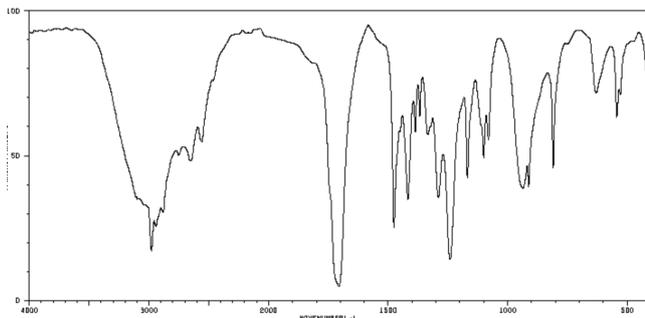
D1 ✗



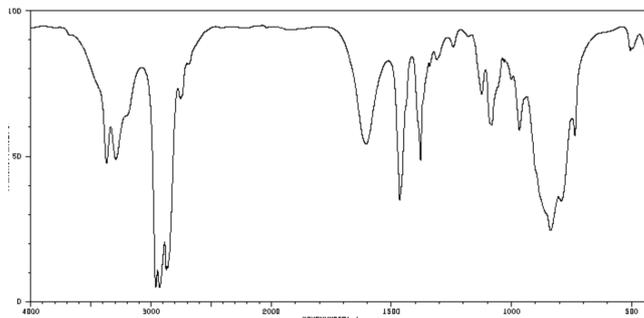
D2 ✗



D3 ✓

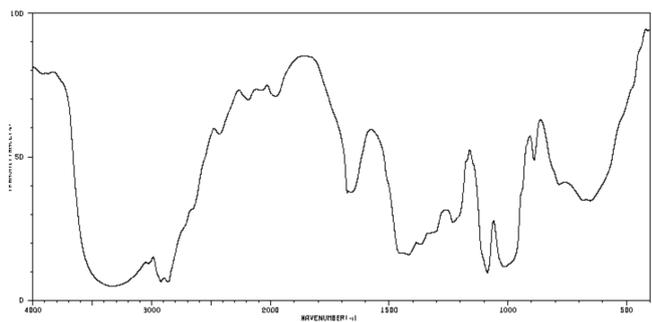


D4 ✗

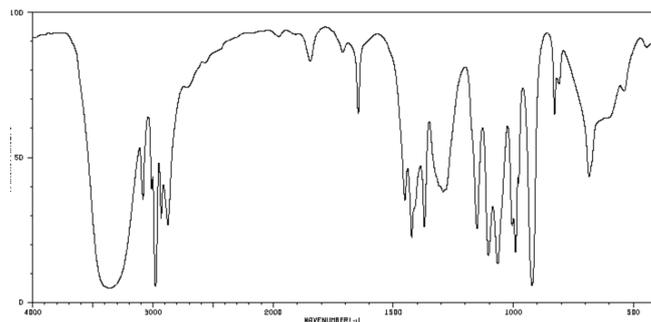


Which of these compounds contain an O–H (alcohol) bond?

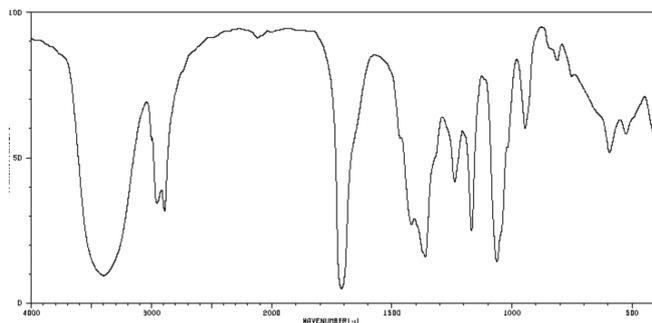
E1 ✓



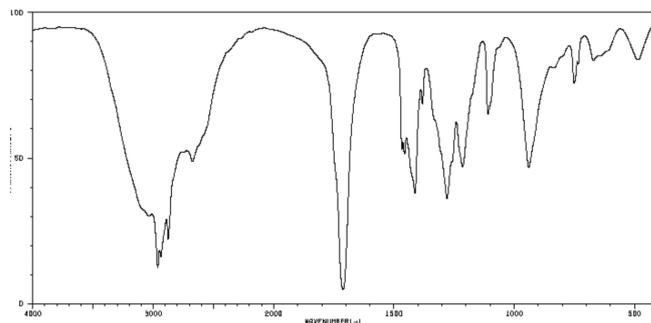
E2 ✓



E3 ✓

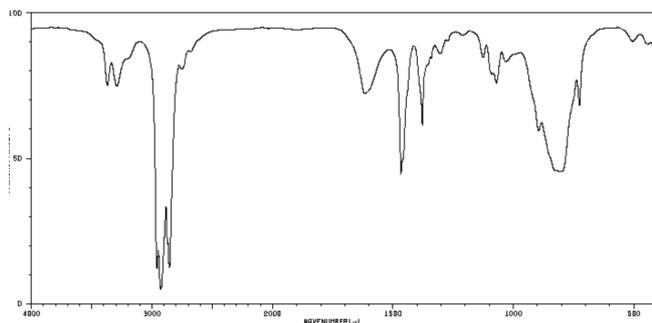


E4 ✗

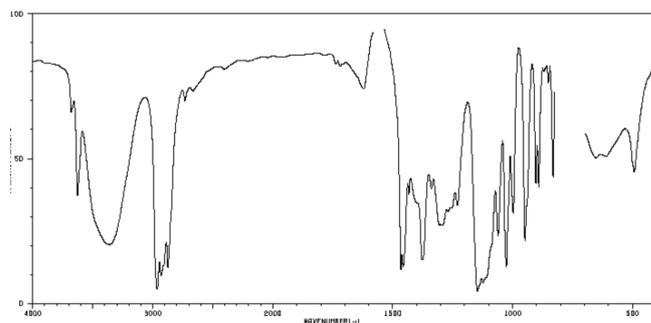


Which of these compounds contain an N–H (amine) bond?

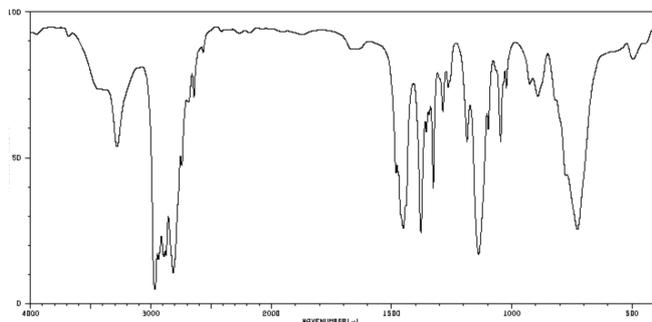
F1 ✓



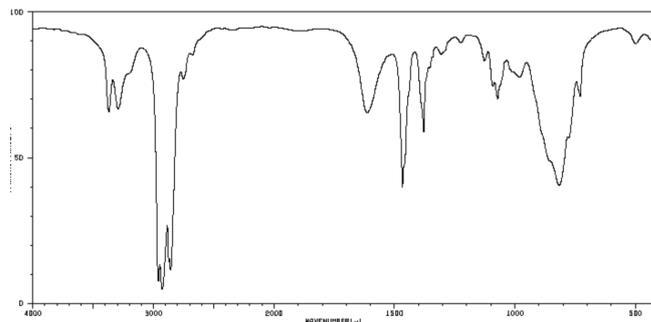
F2 ✗



F3 ✓

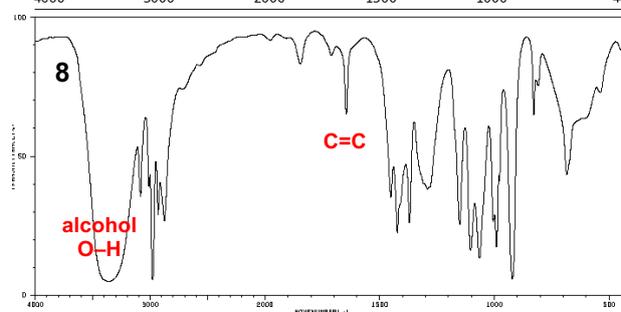
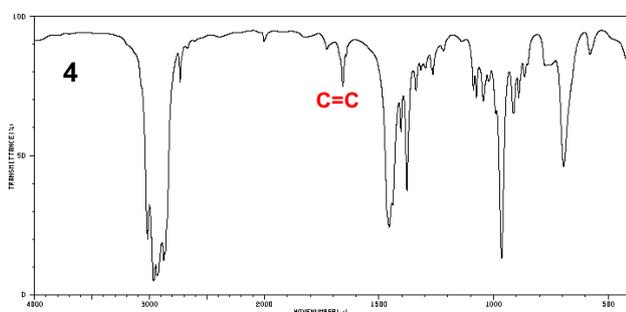
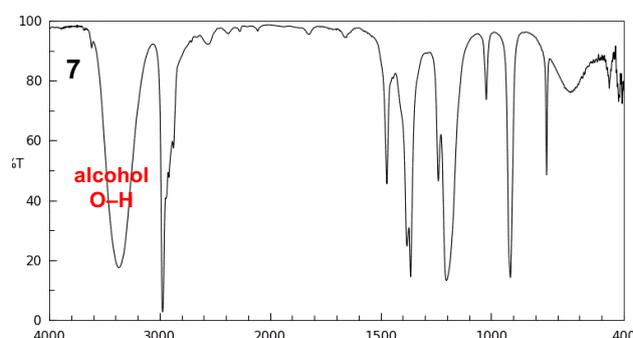
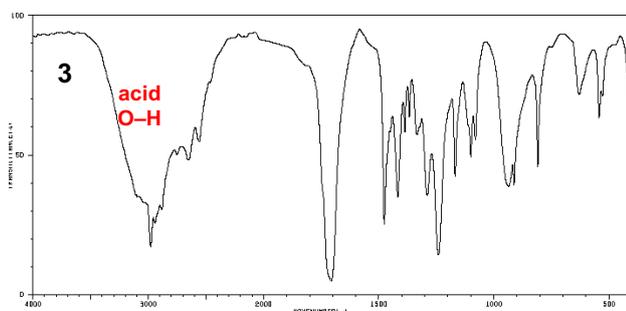
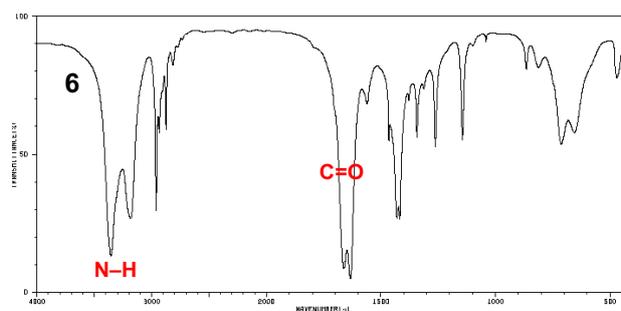
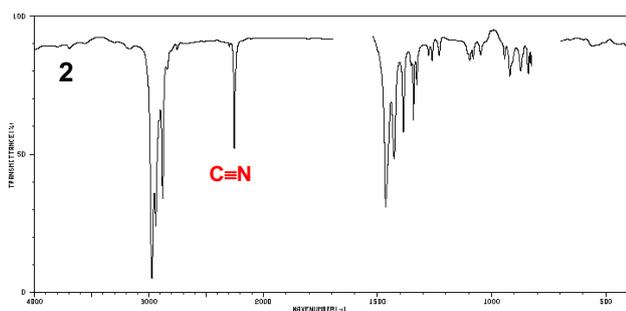
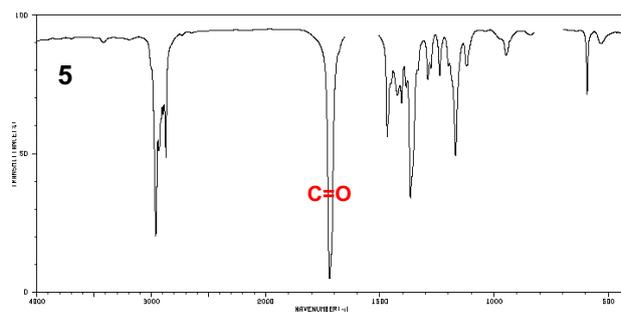
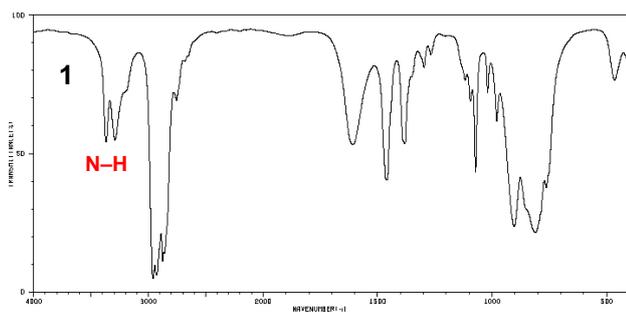


F4 ✓

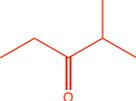
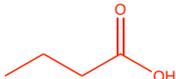


## TASK 3 – IR Problems B

<p><b>5</b></p> $\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_3-\text{CH}_2-\text{CH}-\text{C}-\text{CH}_3 \\    \\ \text{O} \end{array}$	<p><b>8</b></p> $\begin{array}{c} \text{CH}_3-\text{CH}-\text{CH}=\text{CH}_2 \\   \\ \text{OH} \end{array}$	<p><b>3</b></p> $\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_3-\text{CH}-\text{C}-\text{OH} \\    \\ \text{O} \end{array}$	<p><b>7</b></p> $\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_3-\text{C}-\text{CH}_3 \\   \\ \text{OH} \end{array}$
<p><b>4</b></p> $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}_3$	<p><b>1</b></p> $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{NH}_2$	<p><b>6</b></p> $\begin{array}{c} \text{O} \\    \\ \text{CH}_3-\text{CH}_2-\text{CH}_2-\text{C}-\text{NH}_2 \end{array}$	<p><b>2</b></p> $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CN}$



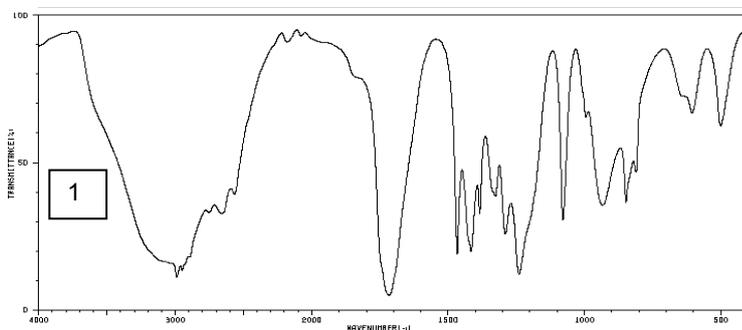
## TASK 4 – IR Problems C

hex-2-ene <b>8</b> 	pentane <b>5</b> 	methylpropan-1-ol <b>3</b> 	2-methylpentan-3-one <b>1/2/6</b> 
butanal <b>1/2/6</b> 	butanoic acid <b>7</b> 	propyl ethanoate <b>1/2/6</b> $\text{CH}_3-\overset{\text{O}}{\parallel}{\text{C}}-\text{O}-\text{CH}_2-\text{CH}_2-\text{CH}_3$	butanenitrile <b>4</b> 

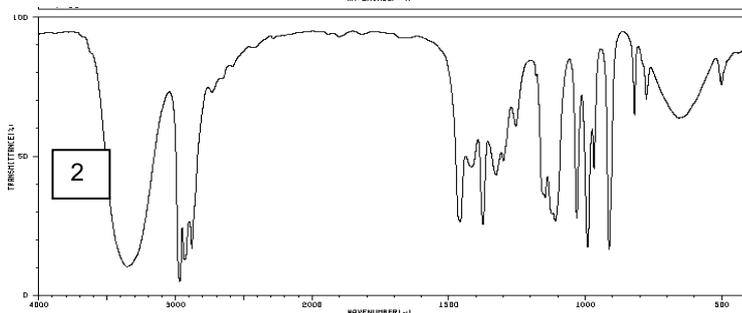
## TASK 5 – IR Problems D

The IR spectra of five compounds are shown. Next to its IR spectrum, draw the structure of the compound and identify by wavenumber and bond the key signals that helped you identify that compound.

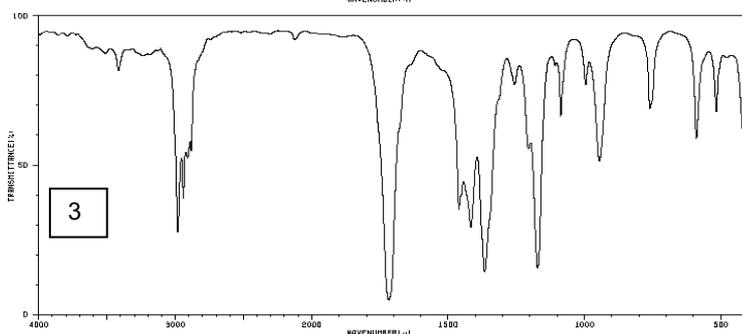
propanoic acid, butanone, 2-methylbut-2-ene, 1-hydroxypropanone, butan-2-ol



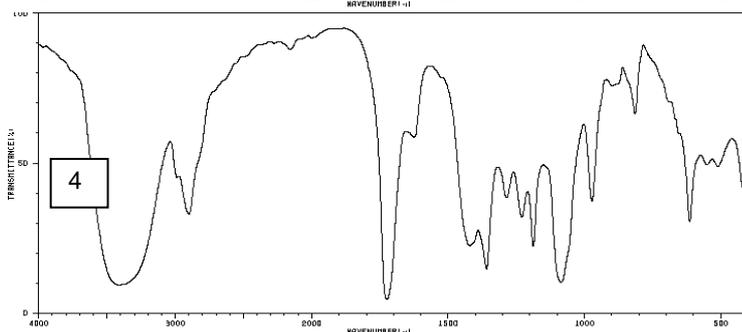
**propanoic acid**  
acid O-H 2500-3000  $\text{cm}^{-1}$



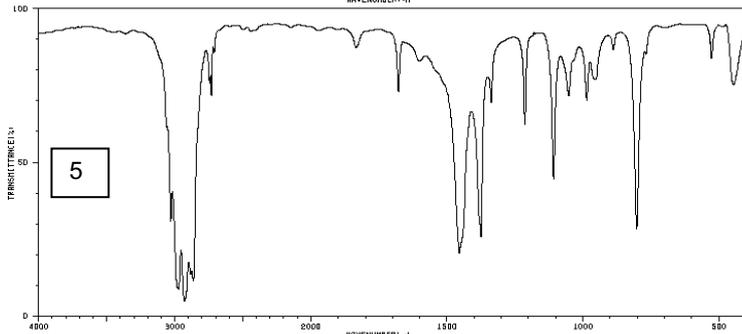
**butan-2-ol**  
alcohol O-H 3230-3550  $\text{cm}^{-1}$



**butanone**  
C=O 1680-1750  $\text{cm}^{-1}$



**1-hydroxypropanone**  
alcohol O-H 3230-3550  $\text{cm}^{-1}$   
C=O 1680-1750  $\text{cm}^{-1}$



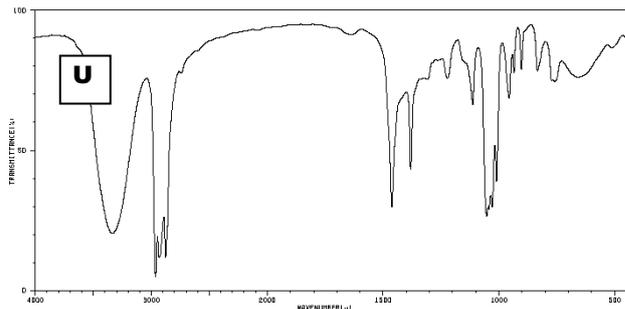
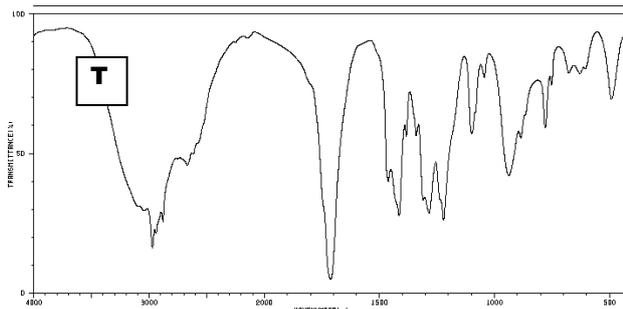
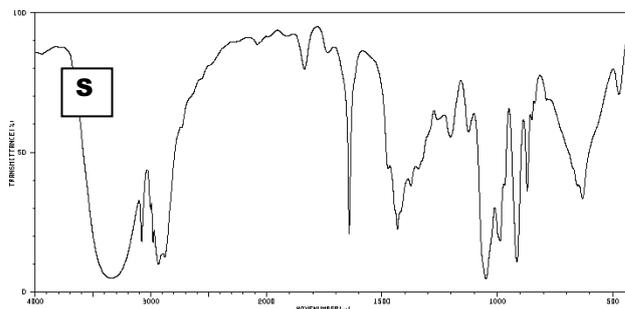
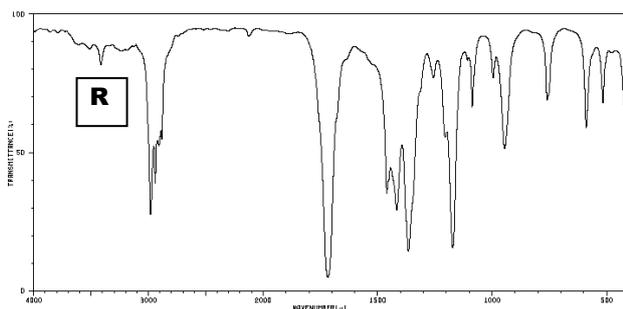
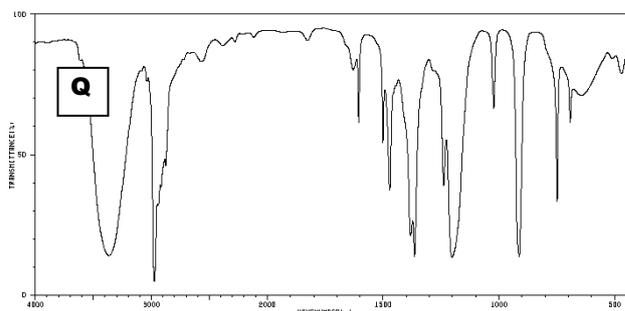
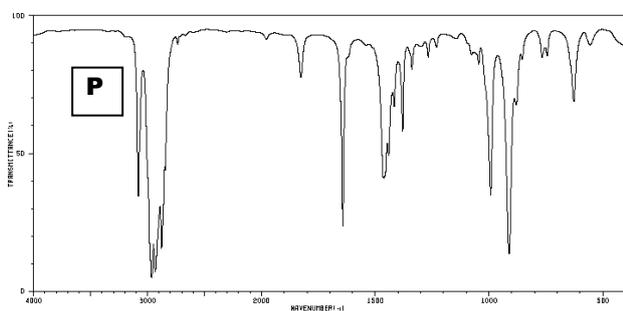
**2-methylbut-2-ene**  
C=C 1620-1680  $\text{cm}^{-1}$

## TASK 6 – IR Problems E

The IR spectra of six compounds are shown. Complete the table to match the spectra to the compounds. Identify any key signals you used to identify each compound. You may not be able to decide between two of the compounds.

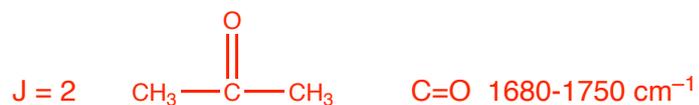
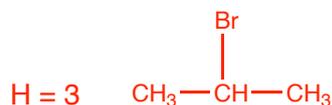
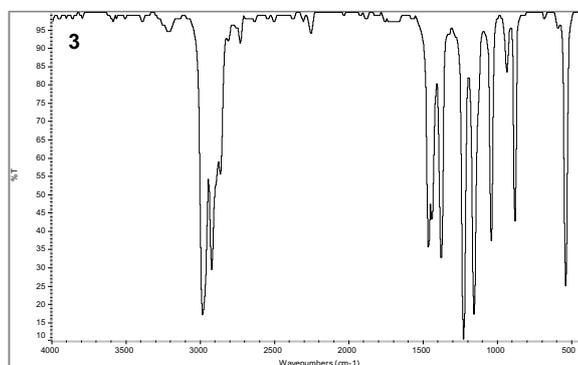
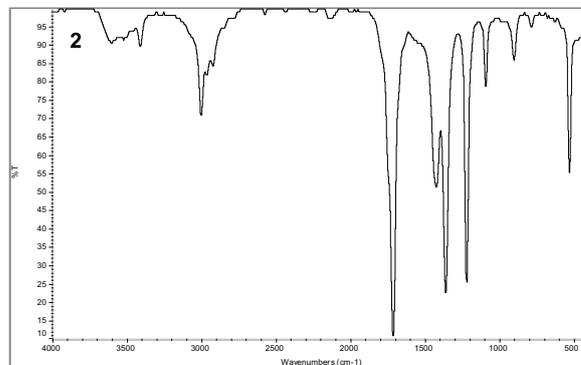
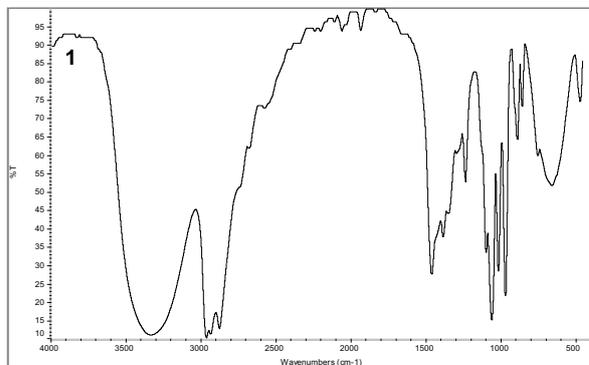
	butanoic acid	butanone	but-3-en-1-ol
Structure	$\text{CH}_3-\text{CH}_2-\text{CH}_2-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	$\text{CH}_3-\text{CH}_2-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_3$	$\text{CH}_2=\text{CH}-\text{CH}_2-\overset{\text{OH}}{\text{CH}_2}$
Spectrum	<b>T</b>	<b>R</b>	<b>S</b>
Bond(s)	<b>O–H (acid)</b>	<b>C=O</b>	<b>C=C</b> <b>O–H (alcohol)</b>
Wavenumber range (cm <sup>-1</sup> )	<b>2500–3000</b>	<b>1680–1750</b>	<b>1620–1680</b> <b>3230–3550</b>

	2-methylpropan-2-ol	2-ethylbutan-1-ol	pent-1-ene
Structure	$\begin{array}{c} \text{OH} \\   \\ \text{CH}_3-\text{C}-\text{CH}_3 \\   \\ \text{CH}_3 \end{array}$	$\begin{array}{c} \text{CH}_3 \\   \\ \text{CH}_2 \\   \quad   \\ \text{CH}_3-\text{CH}_2-\text{CH}-\text{CH}_2 \\   \quad   \\ \text{OH} \end{array}$	$\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}_2$
Spectrum	<b>Q / U</b>	<b>Q / U</b>	<b>P</b>
Bond(s)	<b>O–H (alcohol)</b>	<b>O–H (alcohol)</b>	<b>C=C</b>
Wavenumber range (cm <sup>-1</sup> )	<b>3230–3550</b>	<b>3230–3550</b>	<b>1620–1680</b>



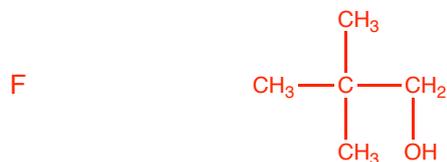
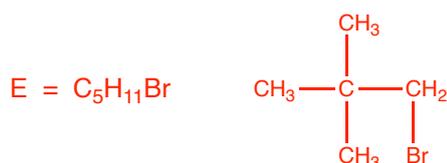
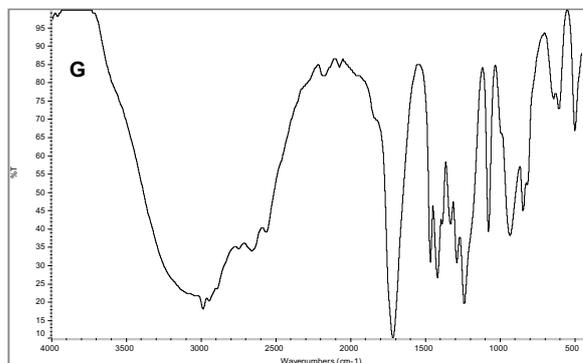
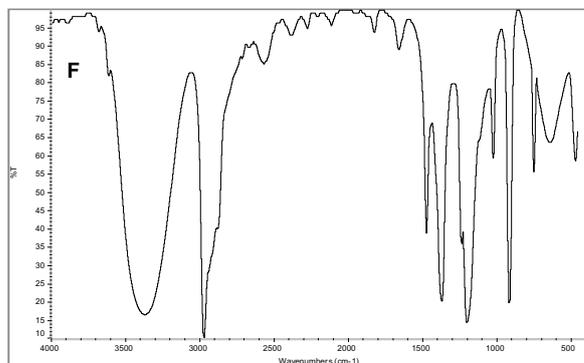
## TASK 7 – IR Problems F

- 1) Propene reacts with HBr to form **H**. **H** reacts with sodium hydroxide to form **I**, and **I** reacts with warm acidified potassium dichromate (VI) to form **J**. The infra-red spectra of **H**, **I** and **J** are given below, but it does indicate which is which. Identify the three compounds **H**, **I** and **J**, using the infra-red spectra below, and decide which spectrum belongs to which compound.



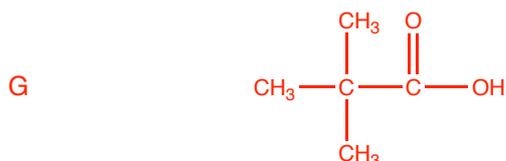
2) Compound **E**, which is a branched chain haloalkane, was found to have the composition by mass of 39.8% C, 7.3% H, and 52.9% Br. There were two peaks for the molecular ions in the spectrum at 150 and 152, of approximately equal intensity. **E** reacts with sodium hydroxide to form **F**, whose infra-red spectrum is shown. **F** does not undergo dehydration with concentrated sulphuric acid.

**F** reacts further with acidified potassium dichromate (VI) to form **G**, whose infra red spectrum is also shown. Draw the structures and name **E**, **F** and **G**. Identify the species responsible for the peaks at 150 and 152 in the mass spectrum of **E**.



alcohol O-H  $3230-3550\text{ cm}^{-1}$

NB - Alcohol **F** cannot dehydrate



acid O-H  $2500-3000\text{ cm}^{-1}$



## TASK 8 – Molecular ion peaks

Compound	Molecule	Mass	Probability	Mass spectrum peaks
CH <sub>3</sub> Br	CH <sub>3</sub> <sup>79</sup> Br	94	$\frac{1}{2}$	2 signals @ 94, 96 in ratio 1:1
	CH <sub>3</sub> <sup>81</sup> Br	96	$\frac{1}{2}$	
CH <sub>2</sub> Br <sub>2</sub>	CH <sub>2</sub> <sup>79</sup> Br <sub>2</sub>	172	$\frac{1}{2} \times \frac{1}{2} = \frac{1}{4}$	3 signals @ 172, 174, 176 in ratio 1:2:1
	CH <sub>2</sub> <sup>79</sup> Br <sup>81</sup> Br	174	$\frac{1}{2} \times \frac{1}{2} = \frac{1}{4}$	
	CH <sub>2</sub> <sup>81</sup> Br <sup>79</sup> Br		$\frac{1}{2} \times \frac{1}{2} = \frac{1}{4}$	
	CH <sub>2</sub> <sup>81</sup> Br <sub>2</sub>	176	$\frac{1}{2} \times \frac{1}{2} = \frac{1}{4}$	
CH <sub>2</sub> BrCl	CH <sub>2</sub> <sup>79</sup> Br <sup>35</sup> Cl	128	$\frac{1}{2} \times \frac{3}{4} = \frac{3}{8}$	3 signals @ 128, 130, 132 in ratio 3:4:1
	CH <sub>2</sub> <sup>79</sup> Br <sup>37</sup> Cl	130	$\frac{1}{2} \times \frac{1}{4} = \frac{1}{8}$	
	CH <sub>2</sub> <sup>81</sup> Br <sup>35</sup> Cl		$\frac{1}{2} \times \frac{3}{4} = \frac{3}{8}$	
	CH <sub>2</sub> <sup>81</sup> Br <sup>37</sup> Cl	132	$\frac{1}{2} \times \frac{1}{4} = \frac{1}{8}$	
CCl <sub>4</sub>	C <sup>35</sup> Cl <sub>4</sub>	152	$\frac{3}{4} \times \frac{3}{4} \times \frac{3}{4} \times \frac{3}{4} = \frac{81}{256}$	5 signals @ 152, 154, 156, 158, 160 in ratio 81 : 108 : 54 : 12 : 1
	C <sup>35</sup> Cl <sub>3</sub> <sup>37</sup> Cl	154	4 ways $\times \frac{3}{4} \times \frac{3}{4} \times \frac{3}{4} \times \frac{1}{4} = \frac{108}{256}$	
	C <sup>35</sup> Cl <sub>2</sub> <sup>37</sup> Cl <sub>2</sub>	156	6 ways $\times \frac{3}{4} \times \frac{3}{4} \times \frac{1}{4} \times \frac{1}{4} = \frac{54}{256}$	
	C <sup>35</sup> Cl <sup>37</sup> Cl <sub>3</sub>	158	4 ways $\times \frac{3}{4} \times \frac{1}{4} \times \frac{1}{4} \times \frac{1}{4} = \frac{12}{256}$	
	C <sup>37</sup> Cl <sub>4</sub>	160	$\frac{1}{4} \times \frac{1}{4} \times \frac{1}{4} \times \frac{1}{4} = \frac{1}{256}$	

## TASK 9 – High-resolution mass spectrometry problems

- 1) 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**

- 2) 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.

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

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

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

- 3) High-resolution mass spectroscopy showed the  $M_r$  of difluoromethane to be 52.0124. The only stable isotope of fluorine is  $^{19}\text{F}$ . Calculate the mass of one atom of  $^{19}\text{F}$  to 4 decimal places.

**$52.0124 - 12.0000 - 2(1.0078) = 37.9968$**

**Mass of  $^{19}\text{F} = \frac{37.9968}{2} = 18.9984$**

- 4) Calculate the accurate mass to 4 decimal places of the two molecular ion peaks in the high-resolution mass spectrum of chloroethane.

**Peak 1  $64.0079$**

**Peak 2  $66.0049$**

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

- a) Calculate the  $M_r$  to 4 decimal places of each of these molecular formulas (which have  $M_r = 102$ ) and then determine the correct molecular formula.

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

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

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

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

b) Identify two possible compounds that have  $M_r = 102.0678$

any 2 of these (there are other possibilities)

