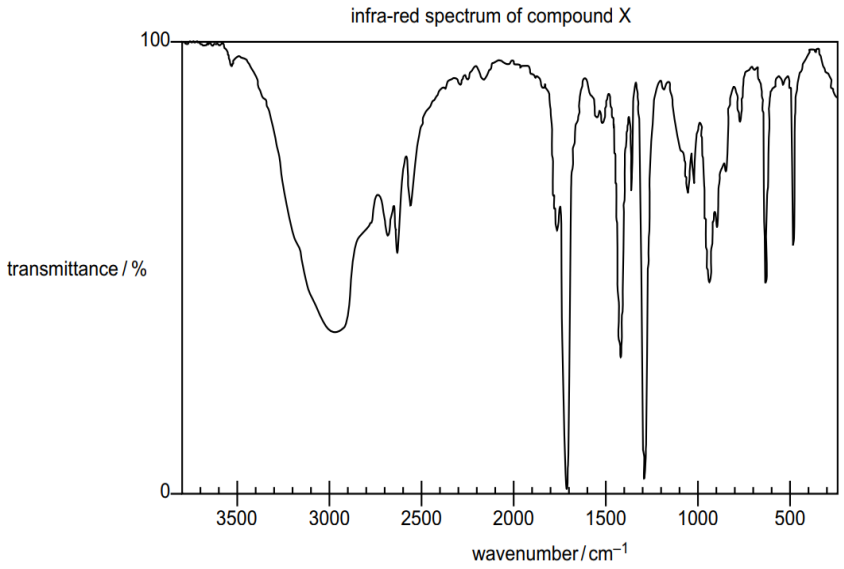
# 22.1 INFRARED SPECTROSCOPY



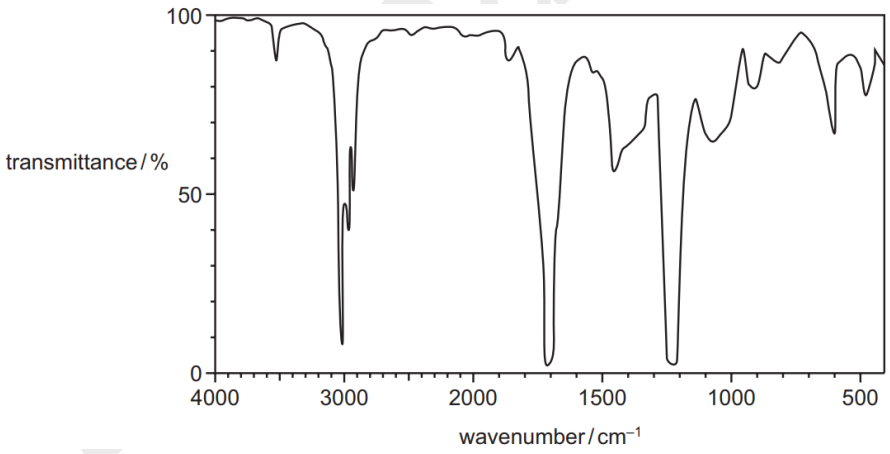
1. Compound X consists of carbon, hydrogen and oxygen only. It has only one functional group.




What can be deduced about X?

**A** X is an aldehyde or ketone.
**B** X is an alcohol.
**C** X is a carboxylic acid.
**D** X is an alkene.

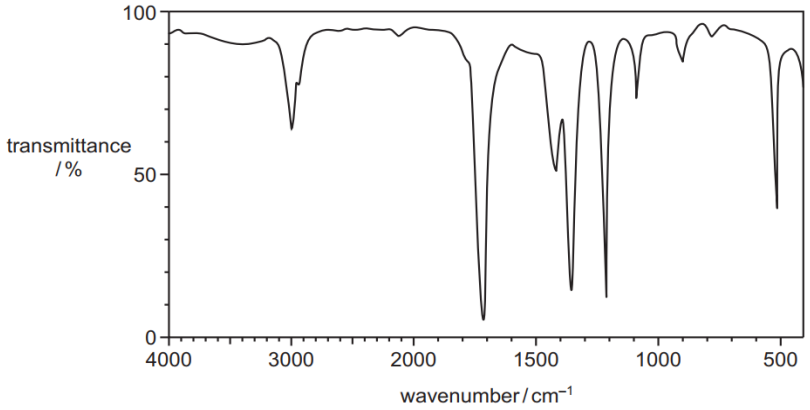
2. The infrared spectrum of a compound is shown.




Which functional group could the compound contain?

A alcohol B carboxylic acid C ester D nitrile

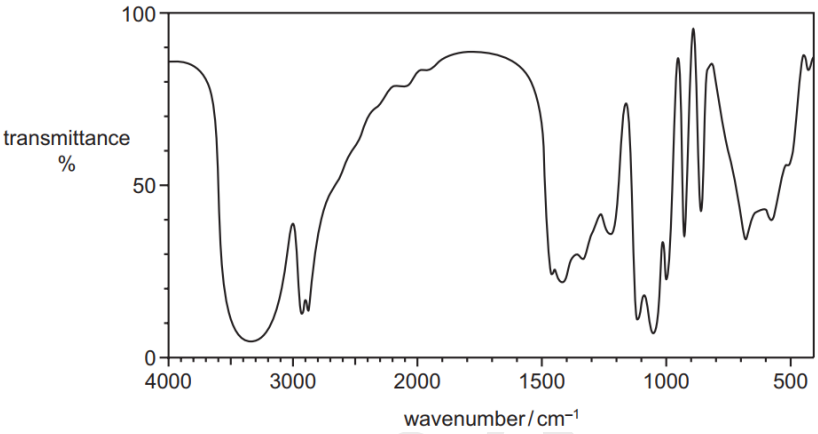
3. The infrared spectrum of an organic compound is shown.




Which compound could give this spectrum?

| | |
|---|---|
| $CH_3CH_2CO_2H$ | **A** |
| $CH_3CH(OH)CH_3$ | **B** |
| $CH_3COCH_3$ | C |
| $CH_3COCH_2OH$ | **D** |

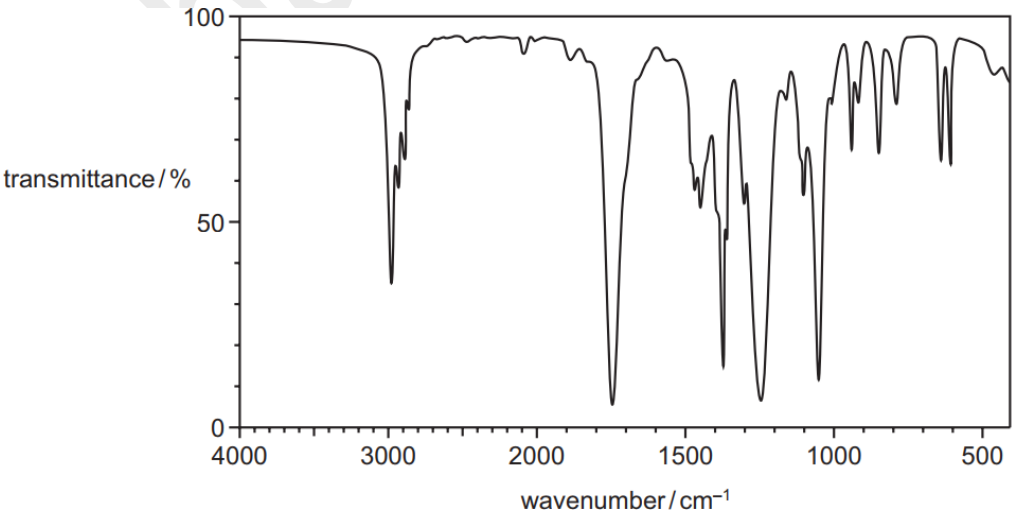
4. The infrared spectrum of compound L is shown




What is the structure of L?

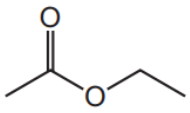
**A** $HOCH_2COCH_2OH$ **B** $HOCH_2CH(OH)CHO$ C $HOCH_2CH(OH)CH_2OH$
**D** $HOCH_2CH_2COOH$

5. Compound X has the empirical formula $C_2H_4O$. Its infra-red spectrum is shown.

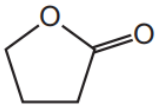



What could be the skeletal formula of compound X?

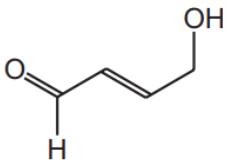
**A**



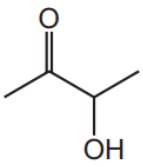
**B**



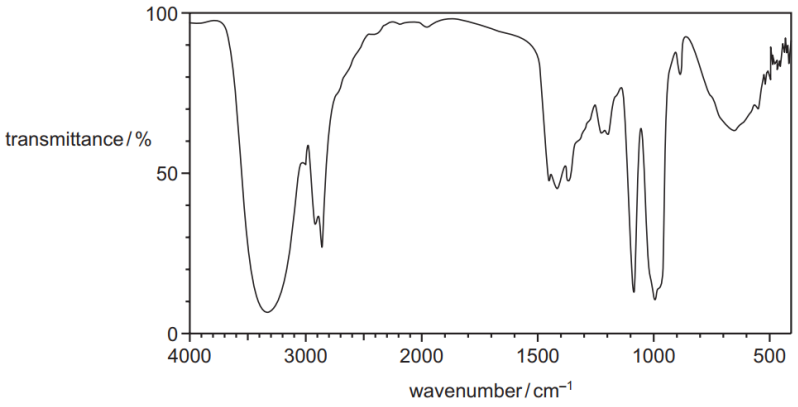
**C**



**D**



6. The infra-red spectrum of Y is shown.




What could Y be?

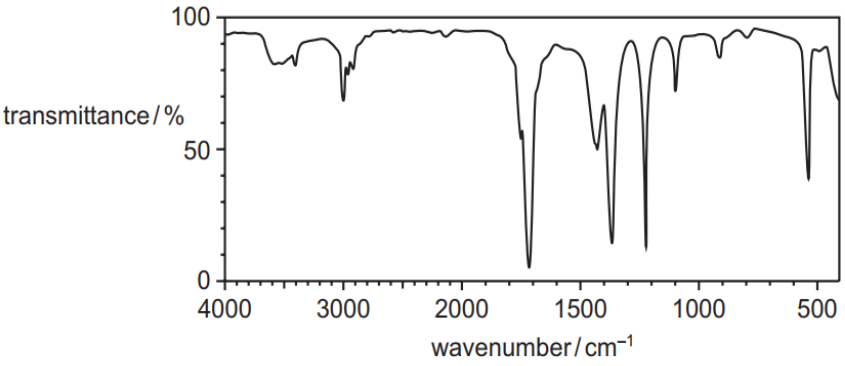
**A** $CH_3CO_2C_2H_5$ **B** $CH_2(OH)CH{=}CHCH_2OH$ **C** $CH_3(CH_2)_2CO_2H$ **D** $CH_2(OH)(CH_2)_2CHO$

7. A molecule of an organic compound, P, contains three carbon atoms and shows a strong absorption at 1720 cm$^{-1}$ in its infrared spectrum.
P is reacted with an excess of hot acidified potassium dichromate(VI) forming organic product Q.
Q shows a strong absorption at 1700 cm$^{-1}$ and a strong, broad absorption centred at 2800 cm$^{-1}$ in its infrared spectrum.
What is P?

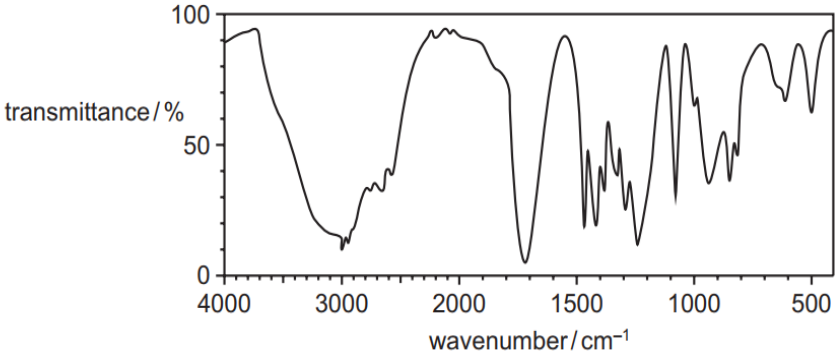
**A** propanal **B** propanone **C** propan-1-ol **D** propan-2-ol

8. The infra-red spectra of three organic compounds are shown.

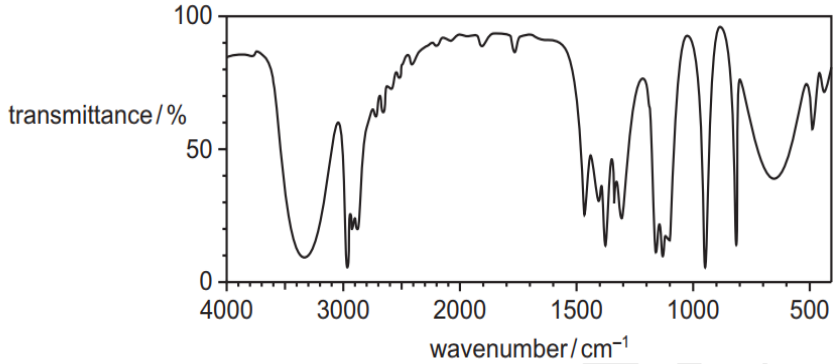
spectrum 1



spectrum 2



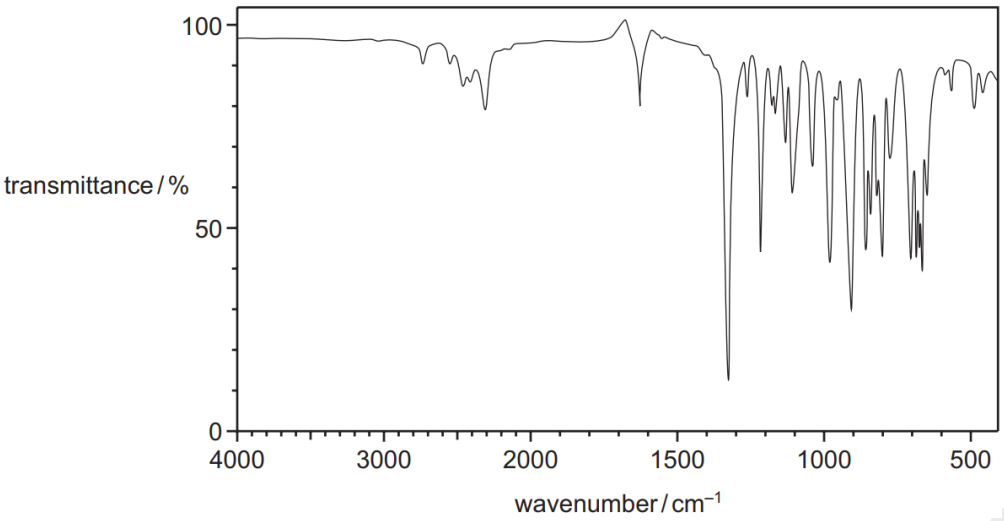

spectrum 3




What could the three compounds be?

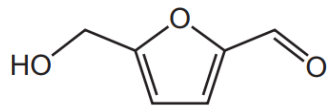
| | spectrum 1 | spectrum 2 | spectrum 3 |
|---|---|---|---|
| **A** | propanoic acid | propanone | propan-2-ol |
| **B** | propanone | propanoic acid | propan-2-ol |
| **C** | propanone | propan-2-ol | propanoic acid |
| **D** | propan-2-ol | propanoic acid | propanone |

9. The infra-red spectrum of molecule Z is shown.

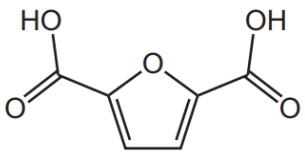



What could be the identity of Z?

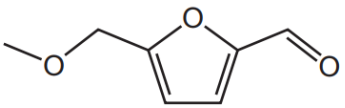
**A**



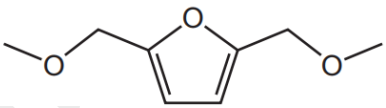

**B**



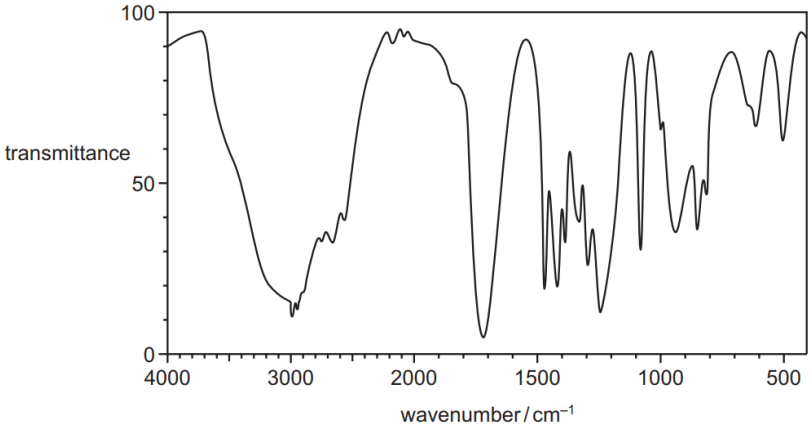

**C**




**D**



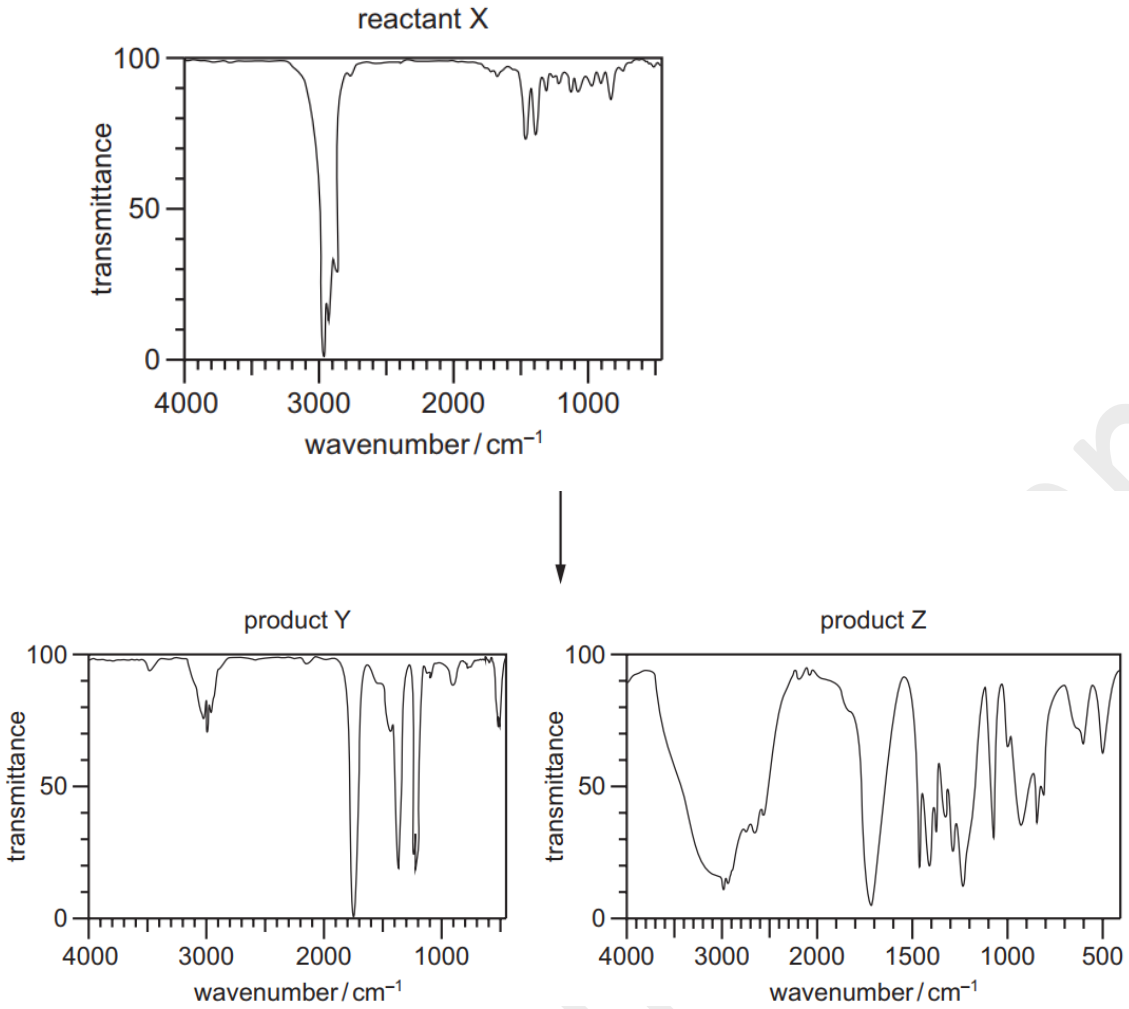

10. Compound X reacts with acidified $K_2Cr_2O_7$ to form compound Y.
The infrared spectrum of compound Y is shown.




What is the identity of compound X?

**A** propan-1-ol
**B** propan-2-ol
**C** propanone
**D** propanoic acid

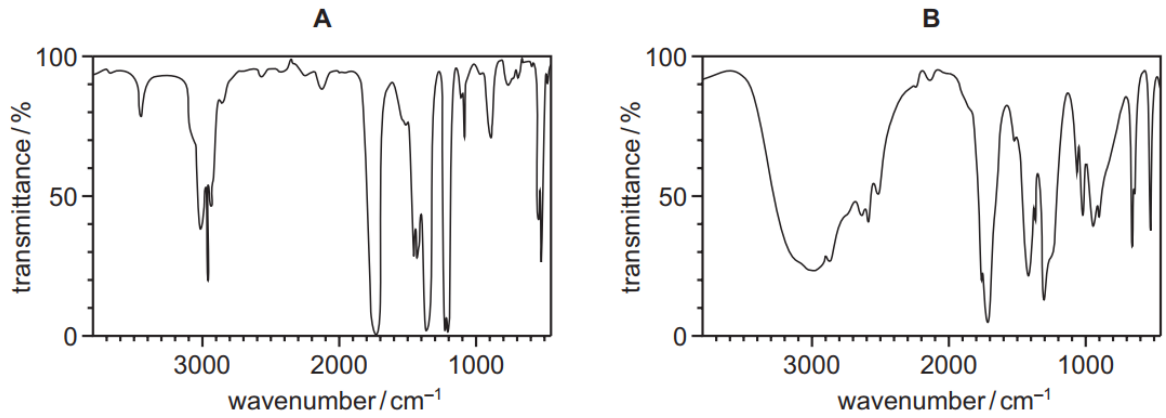
11. When reactant X is treated with a suitable reagent, products Y and Z are formed. Infrared spectra of X, Y and Z are shown.

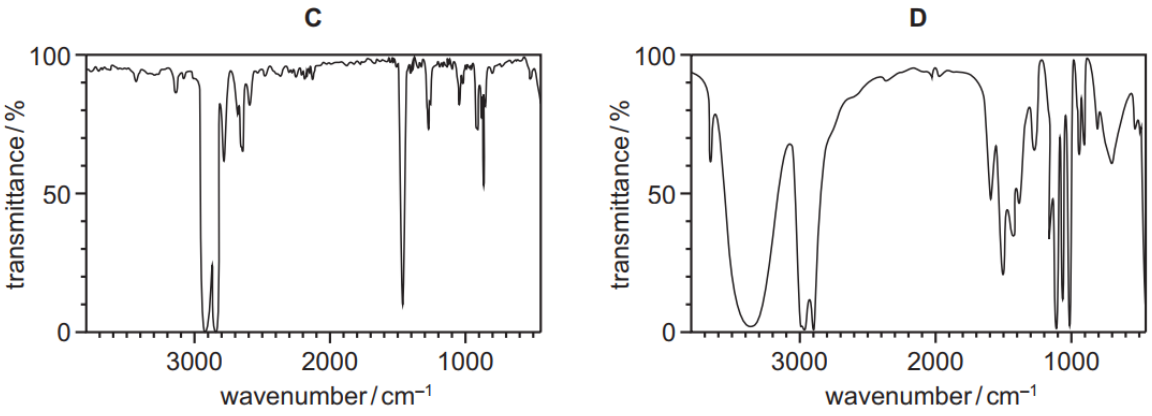



Which row could be correct?

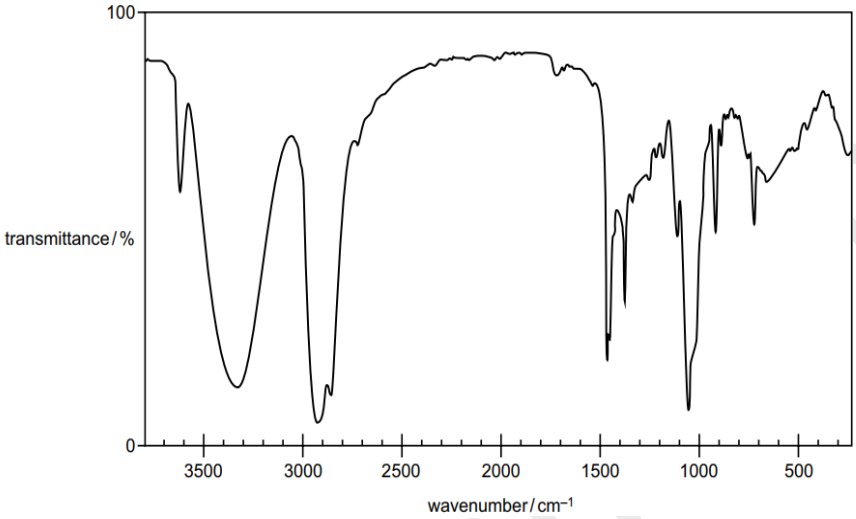
| | X | Y | Z |
|---|---|---|---|
| **A** | 2,3-dimethylpent-2-ene | propanone | butanone |
| **B** | 2-methylpent-2-ene | propanone | propanoic acid |
| **C** | pent-2-ene | ethanoic acid | propanoic acid |
| **D** | propyl propanoate | propan-1-ol | propanoic acid |

12. Which diagram shows the infrared spectrum of a compound that contains both a C=O and an O–H group?



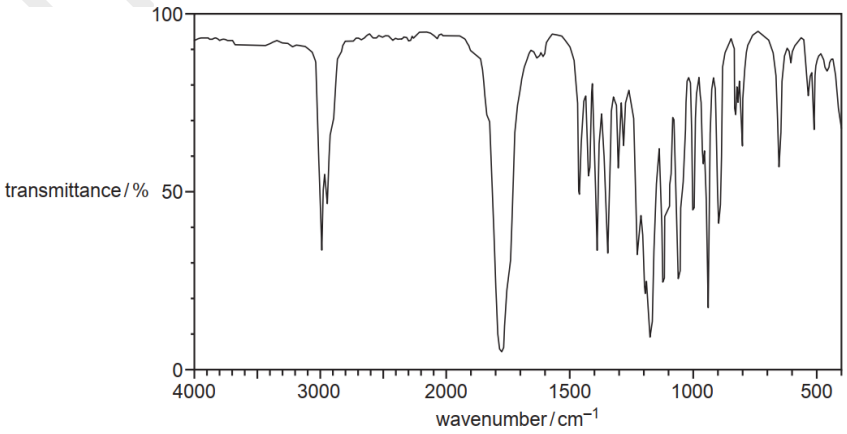



1. The following figure shows the infra-red spectrum of X.

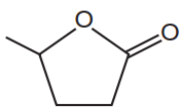



Identify the functional group present in **X** using your answer in **(b)** and information from above figure and following table. Give a reason for your answer.

2. The infrared spectrum of **E** is shown in following chart.

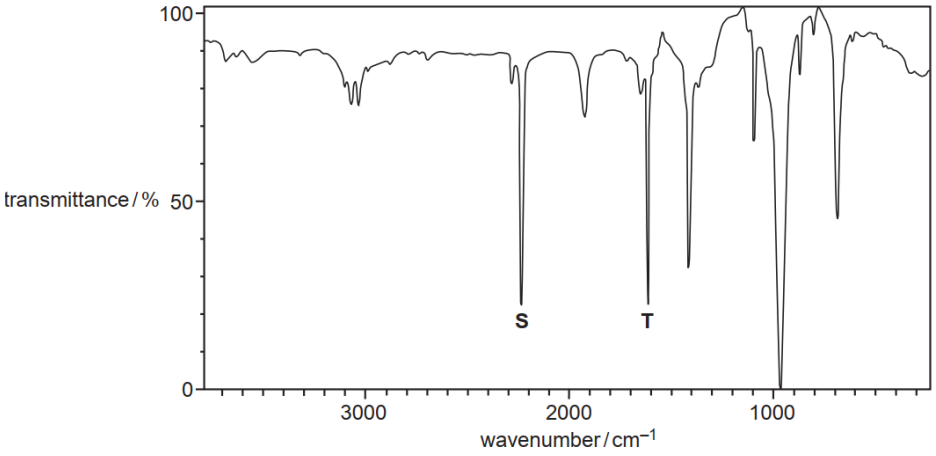



**E**



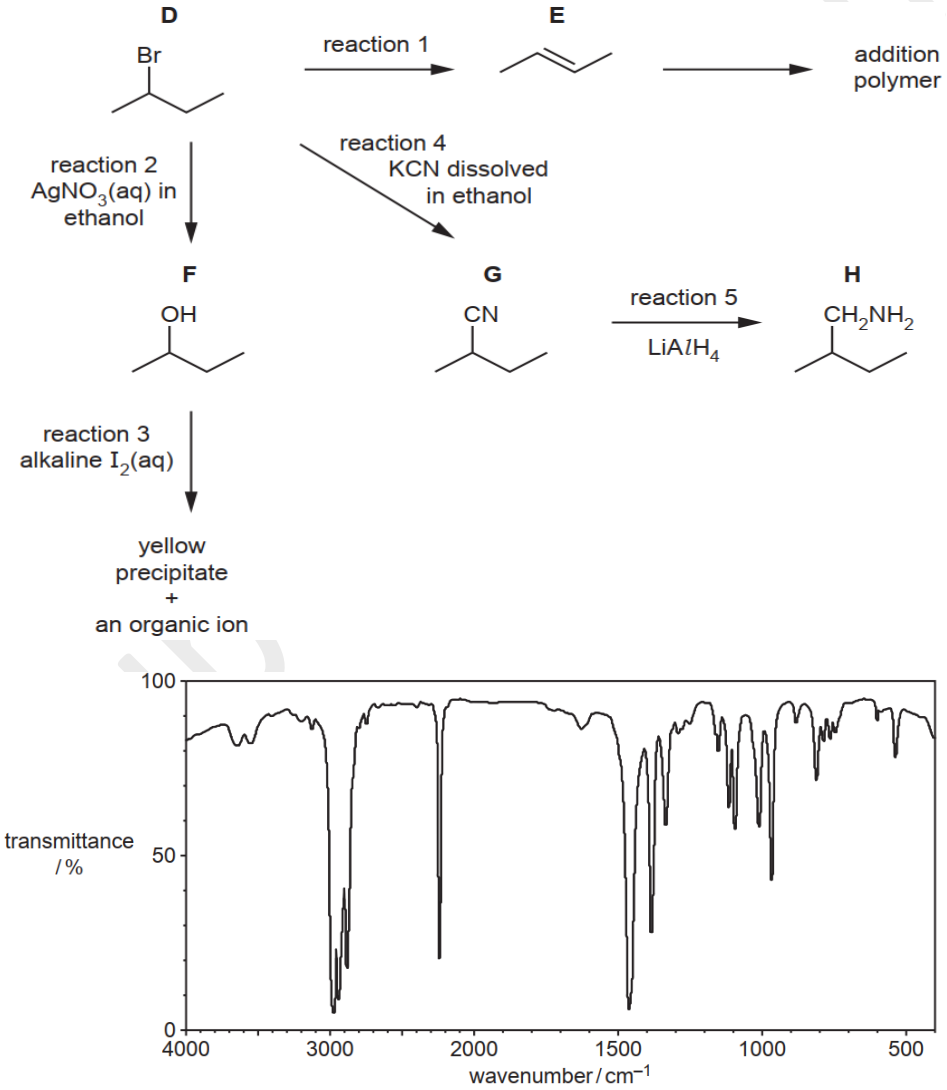
Use above figure and table below to predict **two** differences in the absorptions above 1500cm–1 of the infrared spectrum of **D** compared to **E**. Explain your answer. [2]

3. Fig. 6.3 shows the infrared spectrum of **W**, $CH_2$=CHCN.




Use Table 6.1 to identify the bonds responsible for the absorptions marked **S** and **T** on Fig. 6.3. [1]

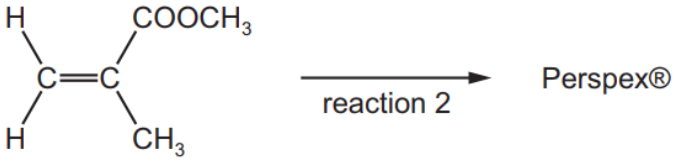
4. The following shows the infrared spectrum of one of the compounds **D**, **E**, **F**, **G** or **H**.




Use information from Table 4.1 (on page 14) to identify which of the compounds **D**, **E**, **F**, **G** or **H** produces the infrared spectrum in Fig. 4.2.
Explain your answer. [2]

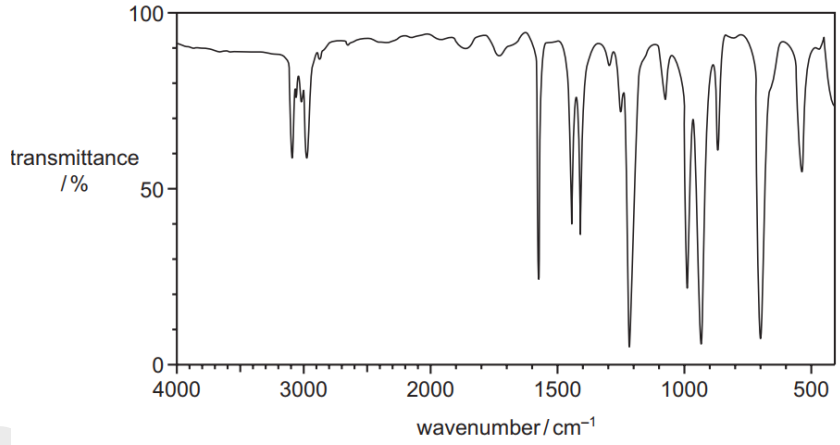
5. M is used to make the addition polymer Perspex®. Use information from Table 4.2 to suggest how the infrared spectra of **M** and Perspex® would differ. Explain your answer. [1]

**M**

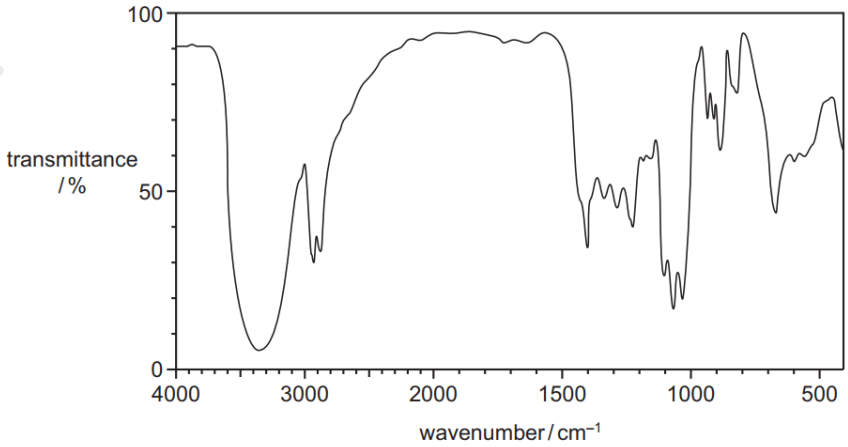



6. Organic compound E contains three carbon atoms.
E reacts with cold dilute acidified KMnO4(aq) to form a single compound F with Mr = 154.9.
Fig. 3.1 shows the infrared spectrum of E.
Fig. 3.2 shows the infrared spectrum of F.

**E**




**F**




Both spectra show absorptions between 2850 and 2950cm–1 owing to C–H bonds in each molecule.
**(i)** Use the two infrared spectra and Table 3.2 to identify the functional group present only in **E**.
Explain your answer, referring only to absorptions at frequencies greater than 1500cm–1. [1]

(ii) Use the infrared spectrum of **F** to identify the functional group formed when **E** reacts with cold dilute acidified KMnO4(aq).
Explain your answer, referring only to absorptions at frequencies greater than 1500cm–1. [1]

(iii) The mass spectrum of **E** shows a molecular ion peak and an M+2 peak of approximately equal abundance at m/e = 120 and 122.

Deduce the relative molecular mass, $M_r$, of **E**. [1]

(iv) Use the information in **3(c)** to suggest a structure for **E**. [1]

(v) Complete the equation for the reaction of **E** with cold dilute acidified $KMnO_4(aq)$ to form **F**.
In the equation, [O] represents cold dilute acidified $KMnO_4(aq)$.

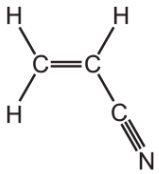
$H_2O$ + [O] + ..... → ..... [1]

7. **P** and **Q** can be detected in the atmosphere by infrared spectroscopy.

**P**

**Q**

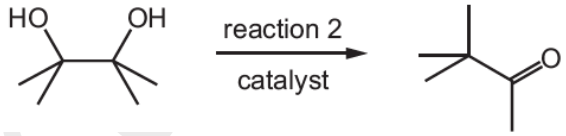
**R**



Identify **two** absorptions, and the bonds that correspond to these absorptions, that will appear in the infrared spectra of both **P** and **Q**. [2]

8. The progress of reaction 2 can be monitored by infrared spectroscopy.

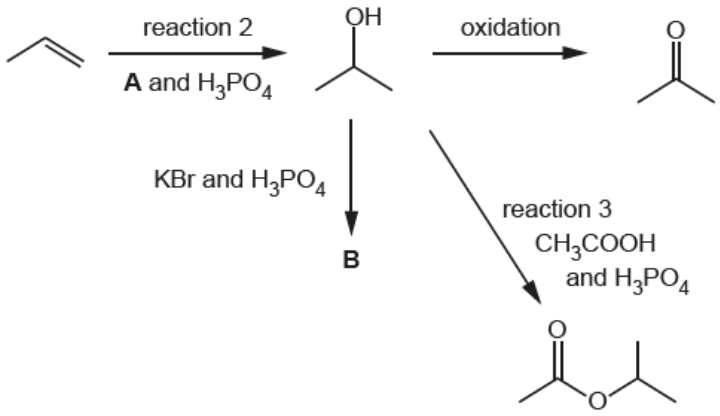
**U**




**V**

The absorption caused by O–H bonds is always present because water is used as a solvent.
Identify two absorptions, and the bonds responsible for these absorptions, whose appearance will change significantly during the reaction. [2]

9. Reaction 3 is monitored using infrared spectroscopy.



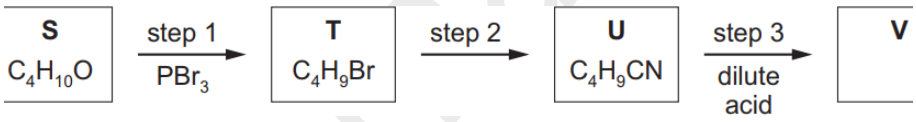

It is not possible to use the O—H absorption frequency to monitor the reaction.
Use Table to identify a suitable bond whose absorption frequency can be used to monitor the progress of reaction 3.
State the change you would see in the infrared spectrum during reaction 3.

bond.....

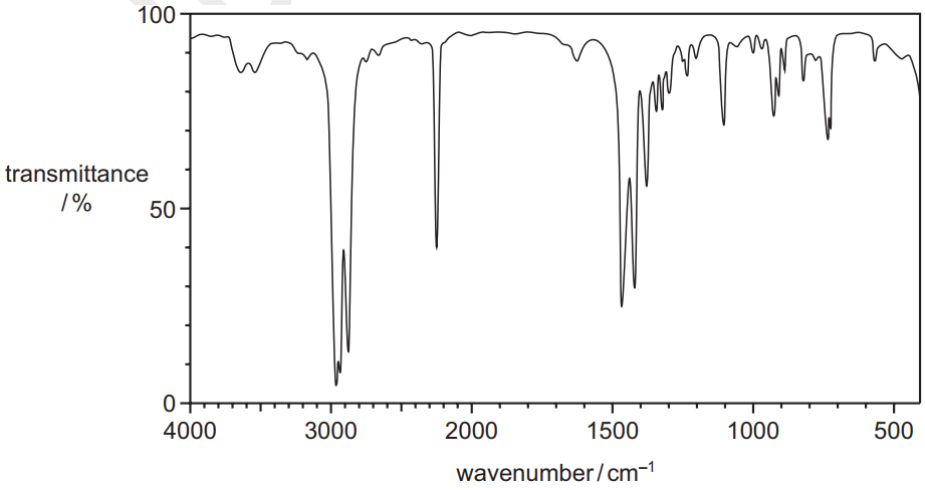
change in infrared spectrum
.....

……
.[2]

10. S is converted to V in a three-step reaction sequence.

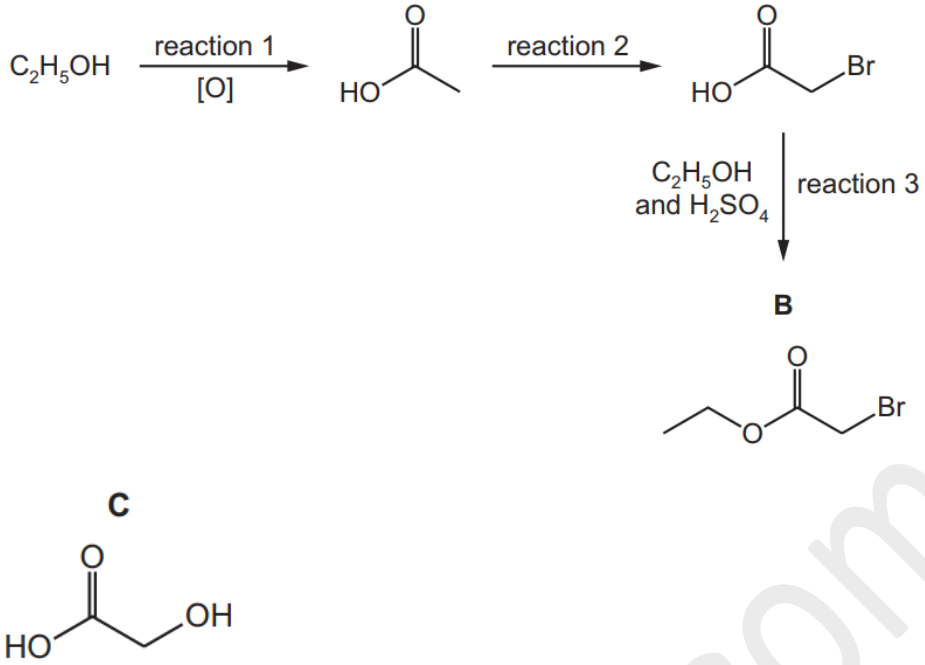



In step 1, the secondary alcohol **S** reacts with $PBr_3$ to produce **T**, which has molecular formula $C_4H_9Br$.
An unlabelled sample contains either **S**, **T** or **U**.
The sample produces the infrared spectrum shown.




Explain how this spectrum confirms that the unknown sample contains **U**.
In your answer identify **one** relevant absorption in the infrared spectrum and the bond that corresponds to this absorption in the region above 1500$cm^{-1}$. [1]

11. Reaction 2 needs to take place in the absence of water to prevent the formation of compound **C**.




**C**




If **C** is present in the reaction mixture of reaction 3, a different compound, compound **D**, will also form.
Compound **D** has two identical functional groups.
The infrared spectrum of **D** shows strong absorptions at 1100cm$^{-1}$ and 1720cm$^{-1}$, but no absorption due to O–H bonds.

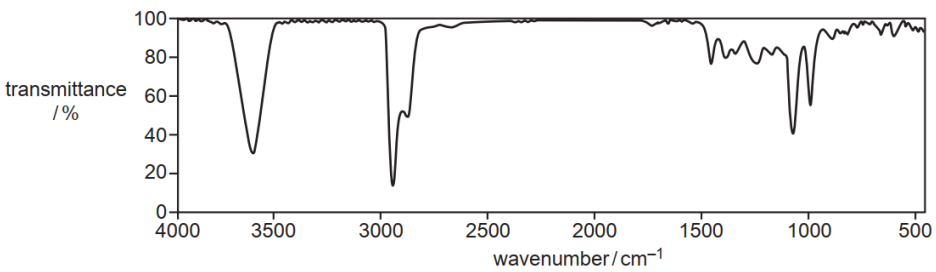
Use the Data Booklet to identify the functional group present in **D**.

Explain your answer as fully as you can. [3]

13. A sample of but-2-enoic acid, $CH_3CH=CHCOOH$, is analysed using infrared spectroscopy.
The infrared spectrum shows a broad peak in the range 2500–3000 cm$^{-1}$.
Which bond is responsible for this peak?

**A** C=C **B** C=O **C** C–O **D** O–H

12. The infrared spectrum of **R** is shown in Fig. 5.3.



Use the absorptions in the region above 1500cm–1 in Table 5.1 when answering this question.
• Add **F** to Fig. 5.3 to identify the peak that is present in an infrared spectrum of both **Q** and **R**. Identify the bond that corresponds to the absorption for **F**.

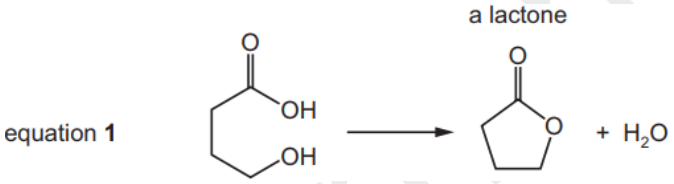
.....

• Add **G** to Fig. 5.3 to identify the peak that is **not** present in an infrared spectrum of **Q**. Identify the bond that corresponds to the absorption for **G**.

.....
[2]

| bond | functional group containing the bond | characteristic infra-red absorption range (in wavenumbers)/cm$^{-1}$ |
|---|---|---|
| C–O | hydroxy, ester | 1040–1300 |
| C=C | aromatic compound, alkene | 1500–1680 |
| C=O | amide<br>carbonyl, carboxyl<br>ester | 1640–1690<br>1670–1740<br>1710–1750 |
| C≡N | nitrile | 2200–2250 |
| C–H | alkane | 2850–3100 |
| N–H | amine, amide | 3300–3500 |
| O–H | carboxyl<br>hydroxy | 2500–3000<br>3200–3650 |

13. Lactones are cyclic esters. Under suitable conditions, lactones form from molecules that have both an alcohol and a carboxylic acid functional group.
Equation **1** shows an example of the formation of a lactone.




The following Figure shows the synthesis of lactone P from compound M.
A student monitors the progress of reaction **2** using infrared spectroscopy.
Use Table 5.1 to suggest why it is difficult to distinguish between **N** and 5-hydroxyhexanoic acid using infrared spectroscopy. [2]

14. Cyclopentene, $C_5H_8$, reacts with hot concentrated acidified $KMnO_4$ to form compound W, $C_5H_8O_4$.
(i) Draw the structure of W. [1]
The infrared spectrum of W is shown in Fig. 3.3.

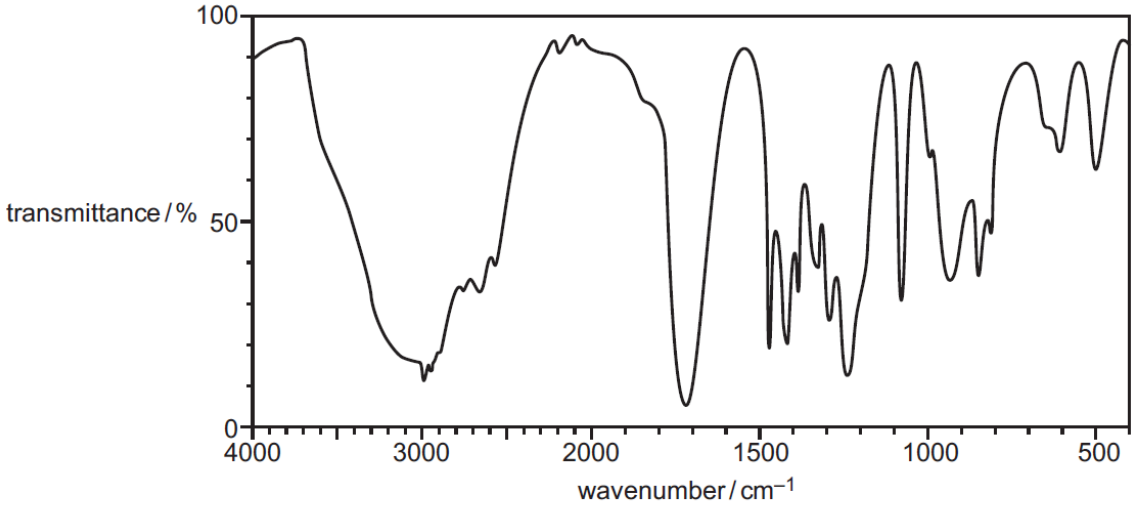



**Fig. 3.3**

15. Identify two absorptions in the infrared spectrum of W that would not be present in the infrared spectrum of cyclopentene.
    • Write 1 or 2 on Fig. 3.3 against each of these two absorptions.
    • Complete Table 3.2 to show which bond is responsible for each absorption that you have identified in Fig. 3.3.

Table 3.2

| absorption | 1 | 2 |
|---|---|---|
| bond responsible | | |

14. The purity of a compound can be determined using infrared spectroscopy.

Propan-2-ol is made by hydration of propene. A sample of the product is obtained.
Which feature of the infrared spectrum of the product would show that no propene remains in the product?

A absorption in the 2900 cm$^{-1}$ region
B strong absorption below 1000 cm$^{-1}$
C the lack of absorption at or near 1250 cm$^{-1}$
D the lack of absorption at or near 1550 cm$^{-1}$

***... ***