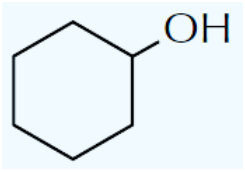
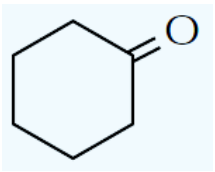
Quiz (Infra-Red Spectroscopy)

1. Give the characteristic wavenumber ranges in the infrared spectrum that would enable you to distinguish between each of the following pairs of compounds.'

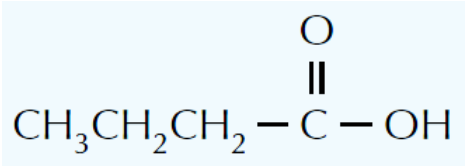
(a)



and



(b)



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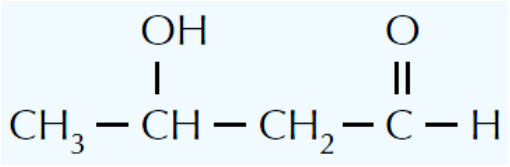
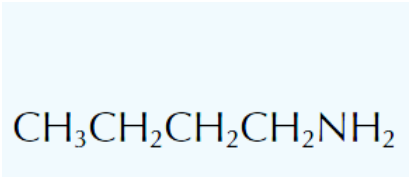


(c)



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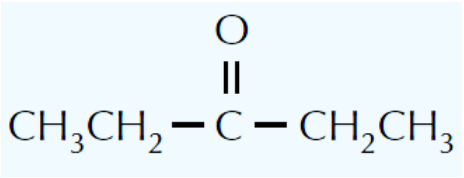
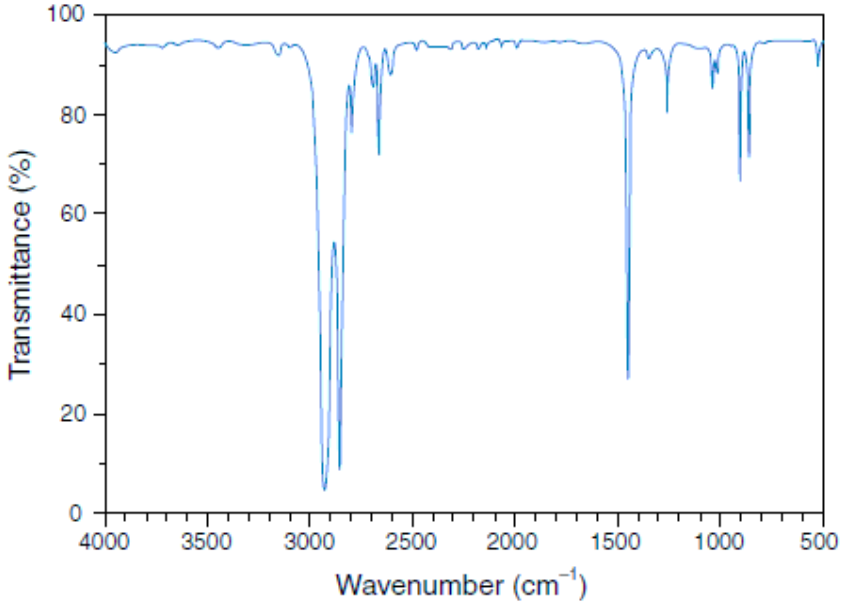


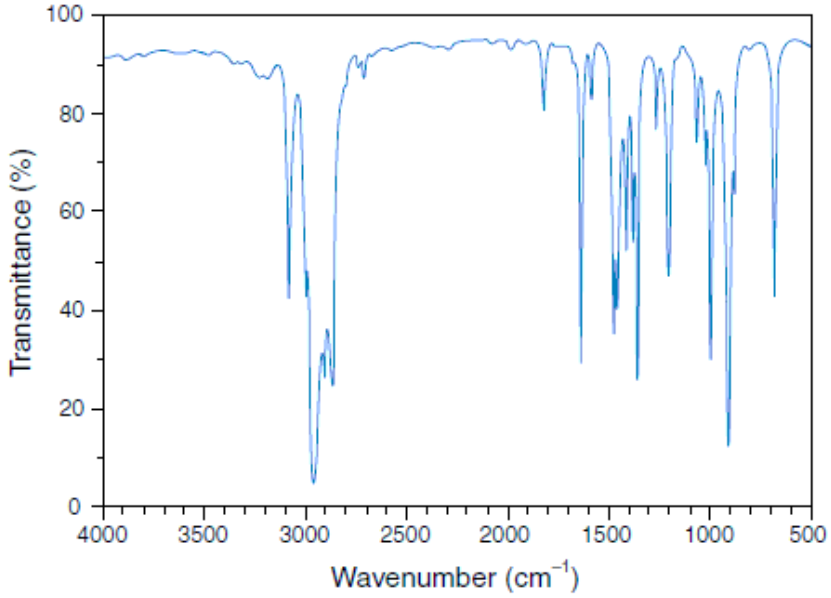
2. By using the correlation table in notes, interpret the following infrared spectra.

(a) Cyclohexane



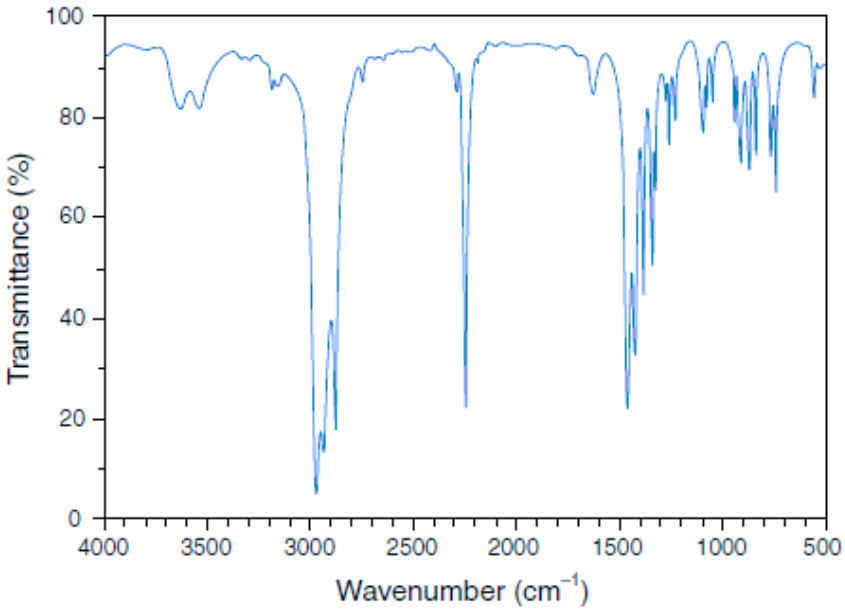
Wavenumber (cm^{-1})	Interpretation
2860 - 2940	

(b) 3,3-dimethylbut-1-ene



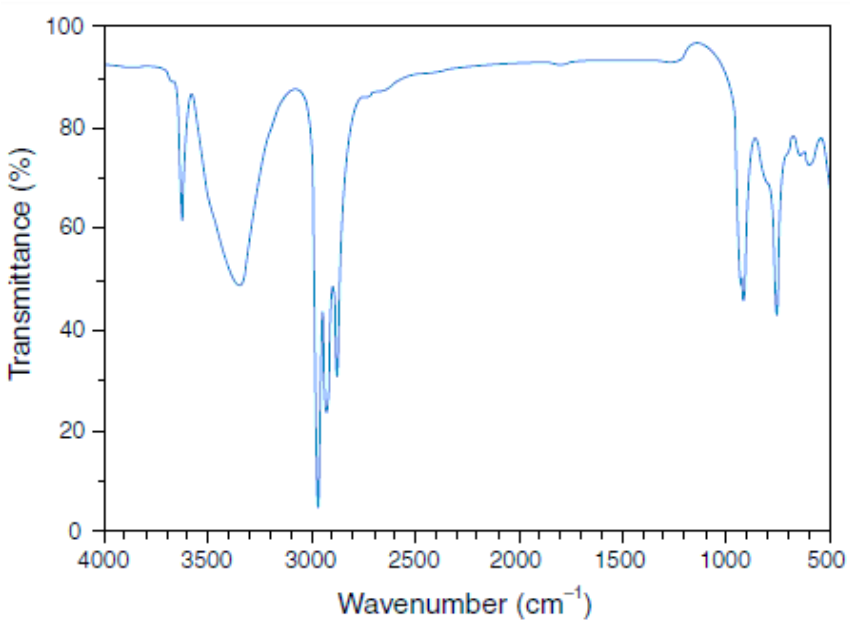
Wavenumber (cm^{-1})	Interpretation
1640	
2860 – 3080	

(c) Butanenitrile



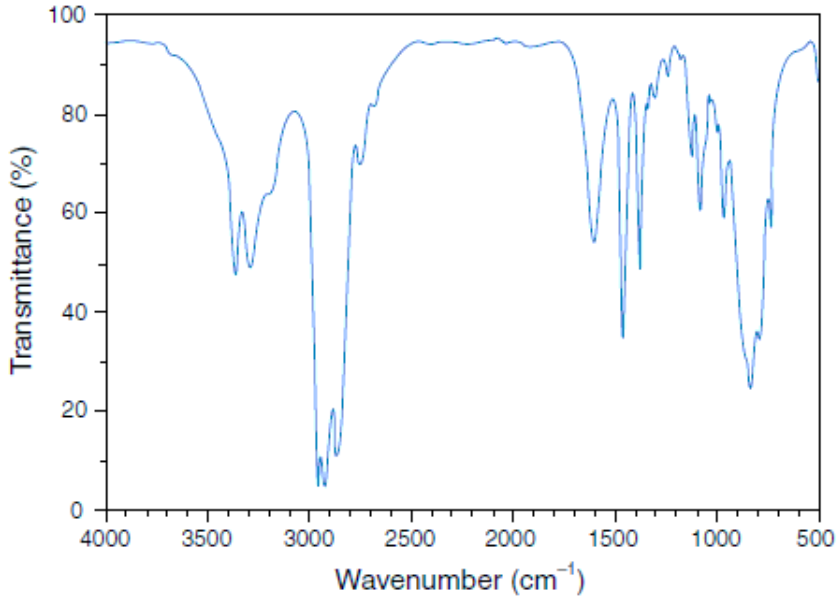
Wavenumber (cm^{-1})	Interpretation
2250	
2880 – 2980	

(d) Butan-2-ol



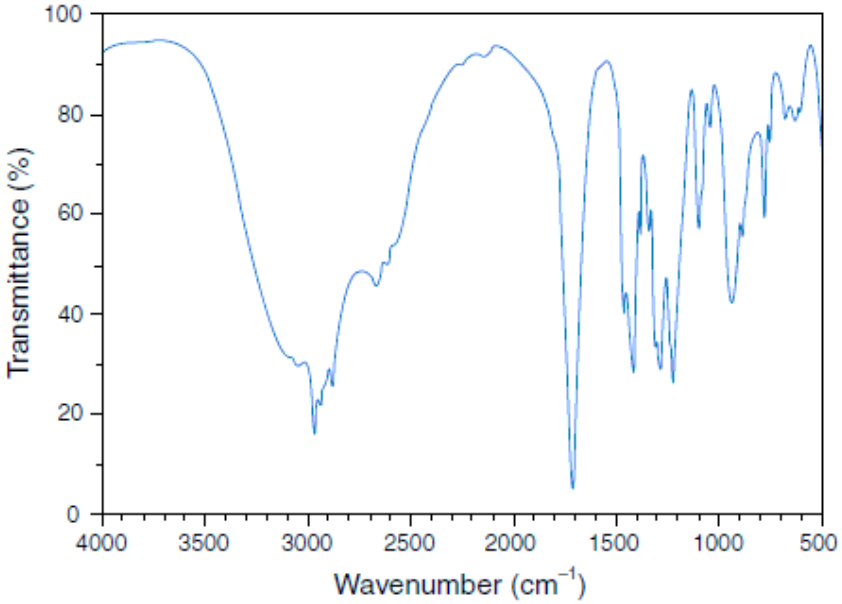
Wavenumber (cm^{-1})	Interpretation
3340	
2880 – 2980	

(e) Butanamine



Wavenumber (cm^{-1})	Interpretation
2880 – 2960	
3370	

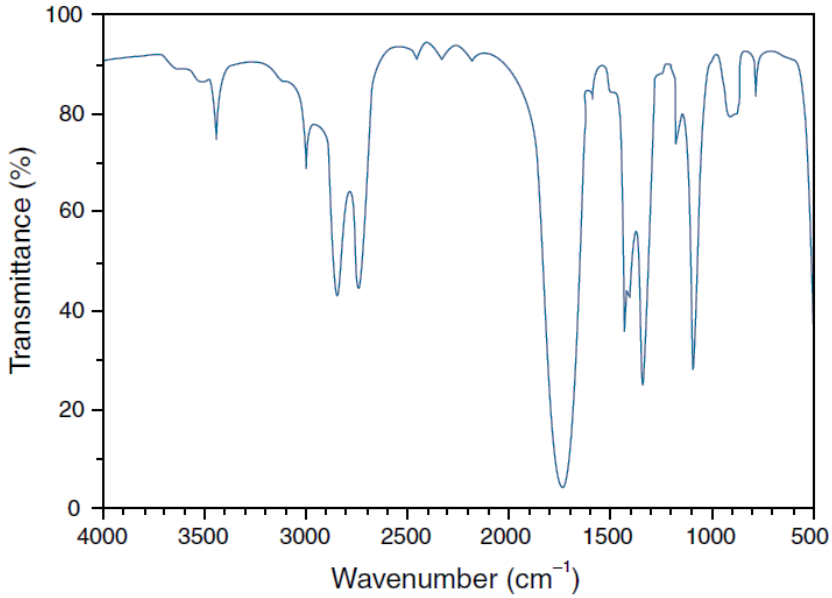
(f) Butanoic acid



Wavenumber (cm^{-1})	Interpretation
1720	
2880 – 2980	
3100	

3. Compound A, with a relative molecular mass of 46.0, has the following composition by mass:

C: 52.18%, H: 13.04%, O: 34.78%

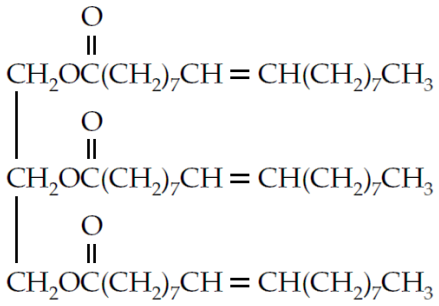


(a) Determine the molecular formula of compound *A*.

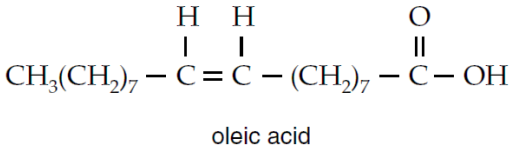
(b) Based on the above information, deduce the structures of compounds *A* and *B*.

(Relative atomic masses: H = 1.0; C = 12.0; O = 16.0)

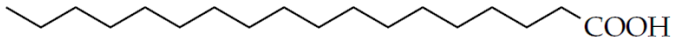
4. Triolein is a triglyceride derived from glycerol and three units of oleic acid. It can be hydrolysed to form oleic acid. Hydrogenation of oleic acid produces stearic acid. The structural formulae of triolein, oleic acid and stearic acid are shown below:



triolein

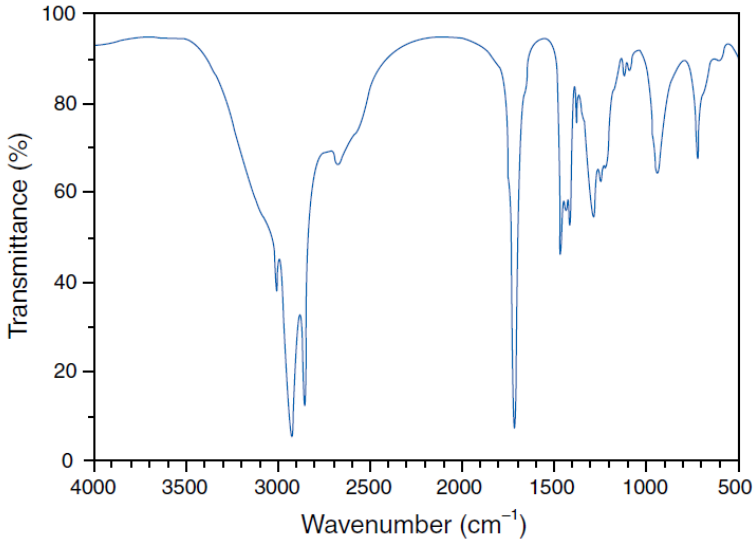


oleic acid



stearic acid

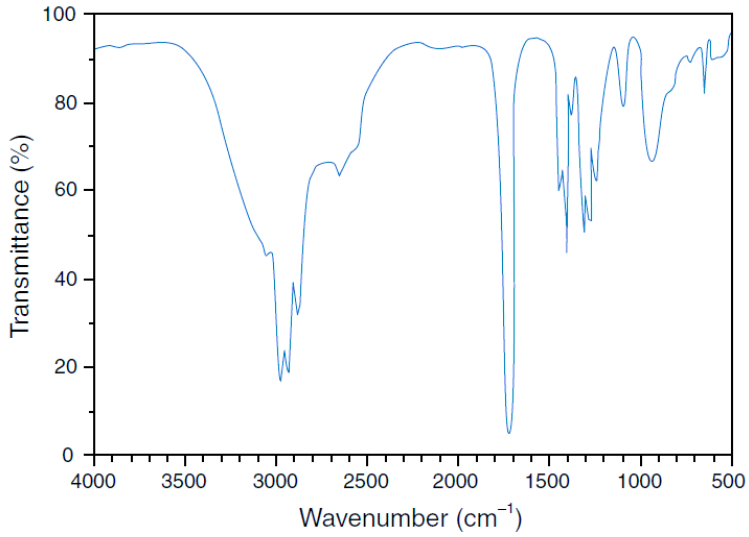
Below is the infrared spectrum of one of the above three compounds.



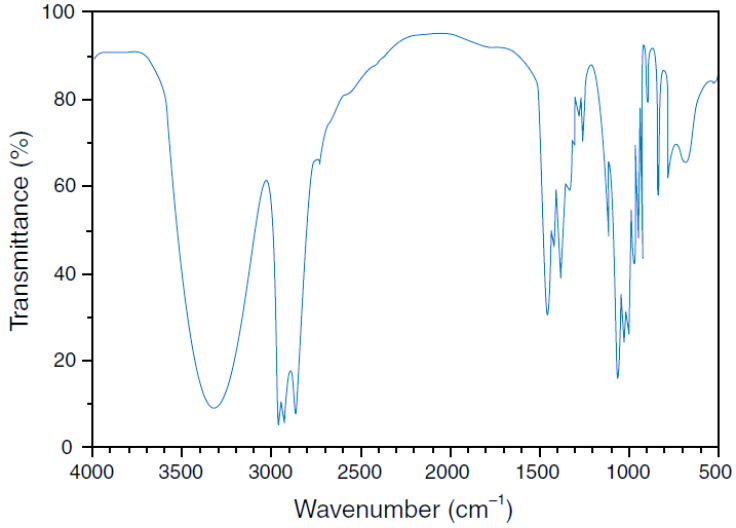
(a) To which of the compounds the above infrared spectrum belongs? Explain your answer.

(b) State TWO limitations of using infrared spectroscopy in identification of functional groups.

5. The infrared spectrum of compound *Y* (with the molecular formula of $C_4H_8O_2$) is shown below. Deduce the possible structures of compound *Y*.

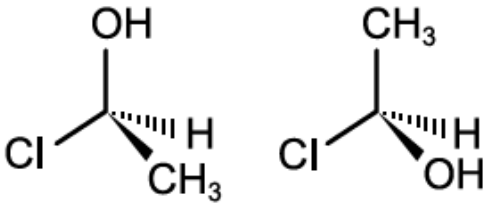


6. Compound *X* contains carbon, hydrogen and oxygen only. 9.20 g of compound *X* burns completely in air to form 17.6 g of carbon dioxide and 10.8 g of water. On vaporization, 2.30 g of compound *X* is found to occupy 1200 cm^3 at room temperature and pressure.
(Relative atomic masses: H = 1.0; C = 12.0; O = 16.0)
(Molar volume of gas at room temperature and pressure = 24.0 $dm^3\ mol^{-1}$)
(a) Determine the empirical formula of compound *X*.
(b) Determine the molecular mass of compound *X*.
(c) Determine the molecular formula of compound *X*.
(d) The IR spectrum of compound *X* is shown below:



Deduce the possible structure of compound *X*.

Remark:
Do you think you can identify the following **enantiomers** with IR spectroscopy?



Since the atoms in enantiomers are linked together in the same order, their infrared spectra should look the same.

Suggested Answer

1. (a) Characteristic wavenumber range 3230 – 3670 cm^{-1} for O—H bond in alcohol; 1680 – 1800 cm^{-1} for C=O bond.

   (b) Characteristic wavenumber range 2500 – 3300 cm^{-1} for O—H bond in carboxylic acid; 3230 – 3670 cm^{-1} for O—H bond in alcohol.

   (c) Characteristic wavenumber range 3350 – 3500 cm^{-1} for N—H bond; 1680 – 1800 cm^{-1} for C=O bond.

2. (a) Cyclohexane

Wavenumber (cm^{-1})	**Interpretation**
2860 - 2940	**C—H bond**

   (b) 3,3-dimethylbut-1-ene

Wavenumber (cm^{-1})	**Interpretation**
1640	**C=C bond**
2860 – 3080	**C—H bond**

   (c) Butanenitrile

Wavenumber (cm^{-1})	**Interpretation**
2250	**C≡N bond**
2880 – 2980	**C—H bond**

   (d) Butan-2-ol

Wavenumber (cm^{-1})	**Interpretation**
3340	**O—H bond**
2880 – 2980	**C—H bond**

   (e) Butanamine

Wavenumber (cm^{-1})	**Interpretation**
2880 – 2960	**C—H bond**
3370	**N—H bond**

   (f) Butanoic acid

Wavenumber (cm^{-1})	**Interpretation**
1720	**C=O bond**
2880 – 2980	**C—H bond**
3100	**O—H bond**

3. (a) Let the mass of compound *A* be 100 g.
Thus, the mass of carbon in the compound = 52.18 g
the mass of hydrogen in the compound = 13.04 g
the mass of oxygen in the compound = 34.78 g

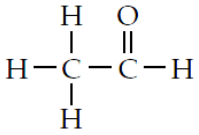
	Carbon	**Hydrogen**	**Oxygen**
Mass (g)	52.18	13.04	34.78
Number of moles (mol)	52.18 / 12.0 = 4.35	13.04 / 1.0 = 13.04	34.78 / 16.0 = 2.17
Mole ratio	4.35 / 2.17 = 2	13.04 / 2.17 = 6	2.17 / 2.17 = 1

$\therefore$ the empirical formula of compound *A* is C_2H_6O.

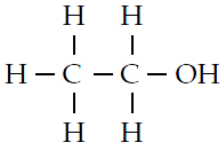
Let the molecular formula of the compound be $(C_2H_6O)_n$.
Relative molecular mass of $(C_2H_6O)_n$ = 46.0
$n \times (12.0 \times 2 + 1.0 \times 6 + 16.0) = 46.0$
$\Rightarrow$ $n = 1$
$\therefore$ the molecular formula of compound *A* is C_2H_6O.

(b) The absence of absorption peak at about 2500 – 3300 cm^{-1} indicates that compound *B* does not contain O–H group.
The absorption peak at 1700 cm^{-1} corresponds to the presence of C=O bond. Compound *B* contains the C=O group. Besides, compound *B* contains only two carbon atoms in its molecule. It is most likely an aldehyde.

$\therefore$ the structure of compound *B* is:



Oxidation of compound *A* gives compound *B*. Thus, compound *A* should be a primary alcohol. The structure of compound *A* is:



4. (a) The infrared spectrum belongs to oleic acid.
The broad absorption peak at around 3100 cm^{-1} corresponds to the presence of the O–H bond of carboxylic acid. Hence, the infrared spectrum does not belong to triolein.

The absorption peak at 1640 cm^{-1} corresponds to the presence of the C=C bond. Hence, the infrared spectrum does not belong to stearic acid.

(b) Some absorption peaks in the spectrum overlap. This may make interpretation difficult.
Interactions between molecules may lead to a complicated pattern of spectrum which is not easy to interpret.

5. The absorption peak at 1720 cm^{-1} corresponds to the presence of C=O bond. Compound Y contains the C=O group.

   The broad absorption peak at 3100 cm^{-1} corresponds to the presence of O—H bond in carboxylic acid. Compound Y contains the —COOH group.

   Possible structures of compound Y:
   $CH_3CH_2CH_2COOH$ OR $(CH_3)_2CHCOOH$

6. (a) Mass of carbon in the CO_2 produced
   = 17.6 x (12.0 / 12.0 + 16.0 x 2)
   = 4.80 g

   Mass of hydrogen in the H_2O produced
   = 10.8 x (1.0 x 2 / 1.0 x 2 + 16.0)
   = 1.20 g

   Mass of oxygen in compound X
   = 9.20 – 4.80 – 1.20
   = 3.20 g

	Carbon	**Hydrogen**	**Oxygen**
Mass (g)	4.80	1.20	3.20
Number of moles (mol)	4.80 / 12.0 = 0.40	1.20 / 1.0 = 1.20	3.20 / 16.0 = 0.20
Mole ratio	0.40 / 0.20 = 2	1.20 / 0.20 = 6	0.20 / 0.20 = 1

   ∴ empirical formula of compound X is C_2H_6O.

   (b) Number of moles of 2.30 g of compound X
   = 1.2 / 24.0
   = 0.05

   Molar mass of compound X
   = 2.30 / 0.05
   = 46.0 g mol^{-1}

   ∴ molecular mass of compound X is 46.0.

   (c) Let the molecular formula of compound X be $(C_2H_6O)_n$
   $n \times (12.0 \times 2 + 1.0 \times 6 + 16.0) = 46.0$
   ⇒ $n = 1$
   ∴ the molecular formula of compound *X* is C_2H_6O.

   (d) A broad absorption peak at 3320 cm^{-1} corresponds to the presence of O—H bond in alcohol. Compound X contains the O—H group.
   Possible structure of compound X: CH_3CH_2OH