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EXPERIMENT NO. 5

AIM:

To analyse the given IR spectra and identify the functional groups on the basis of the peaks in the corresponding spectrum.

REQUIREMENTS: IR spectra.

THEORY:

- Infrared spectroscopy is the study of the interaction of infrared light with matter. The fundamental measurement obtained in infrared spectroscopy is an infrared spectrum, which is a plot of measured infrared intensity versus wavelength (or frequency) of light.

$$c = \nu\lambda$$

$$W = \frac{1}{\lambda}$$

These show that light waves may be described by their frequency, wavelength or wavenumber.

- When a molecule absorbs infrared radiation, its chemical bonds vibrate. The bonds can stretch, contract and bend. Fortunately, the complex vibrational motion of a molecule can be broken down into a no. of constituents vibrations called normal modes. Different molecules vibrate at different frequencies because their structures are diffent and hence they can be distinguished using infrared spectroscopy.

- 1. $\frac{\partial \mu}{\partial x} \neq 0$ — (1)

$\partial\mu$ = change in dipole moment

∂x = change in bond distance

The first necessary condition for a molecule to absorb infrared light

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• Table of IR absorptions

Functional Group		Characteristic Absorption (cm^{-1})
• Alkyl	C–H stretch	2950 – 2850
• Alkenyl	C–H stretch	3100 – 3010
Alkenyl	C=C stretch	1680 – 1620
• Alkynyl	C–H stretch	~3300
Alkynyl	C≡C stretch	2260 – 2100
• Aromatic	C–H stretch	~3030
Aromatic	C–H Bending	860 – 680
Aromatic	C=C Bending	1700 – 1500
• Alcohol / Phenol	O–H stretch	3350 – 3200
• Carboxylic Acid	O–H stretch	3000 – 2500
• Amine	N–H stretch	3500 – 3300
• Nitrile	C≡N stretch	2260 – 2220
• Aldehyde	C=O stretch	1740 – 1690
Ketone	C=O stretch	1750 – 1680
Ester	C=O stretch	1750 – 1735
Carboxylic Acid	C=O stretch	1780 – 1710
Amide	C=O stretch	1690 – 1630
• Amide	N–H stretch	3700 – 3500

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is that the molecule must have a vibration during which the change in dipole moment w.r.t. distance is non-zero.

2. $\Delta E_{vib.} = hc\bar{\nu}$

$\bar{\nu}$ = wavenumber in cm^{-1}

c = speed of light in cm/sec.

The second necessary condition, is that energy of light impinging on a molecule must equal a vibrational energy level difference within the molecule

- The frequency of light that a molecule will absorb, and is the frequency of vibration of normal mode excited by that light is given by -

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$$

k = force constant (in N/cm)

ν = frequency (in cm^{-1})

μ = reduced mass in kg

- No two chemical substances in the universe have the same force constants and atomic masses, which is why infrared spectrum of each chemical substance is unique.
- The different vibrations of different functional groups in the molecule give rise to bands of differing intensity. This is because $\partial\mu/\partial x$ is different for each of these vibrations.
- In any sample, where hydrogen bonding occurs, the no. and strength of intermolecular interaction varies greatly within the sample, causing the bands in these samples to be particularly broad.

PROCEDURE:

Analyse the given IR spectra from the table of IR absorptions, and write down the functional groups.

RESULT:

In IR spectrum (A), the peak corresponds to carbonyl group, (>c=o) in 1750 - 1680 cm^{-1}, thus representing a ketone.

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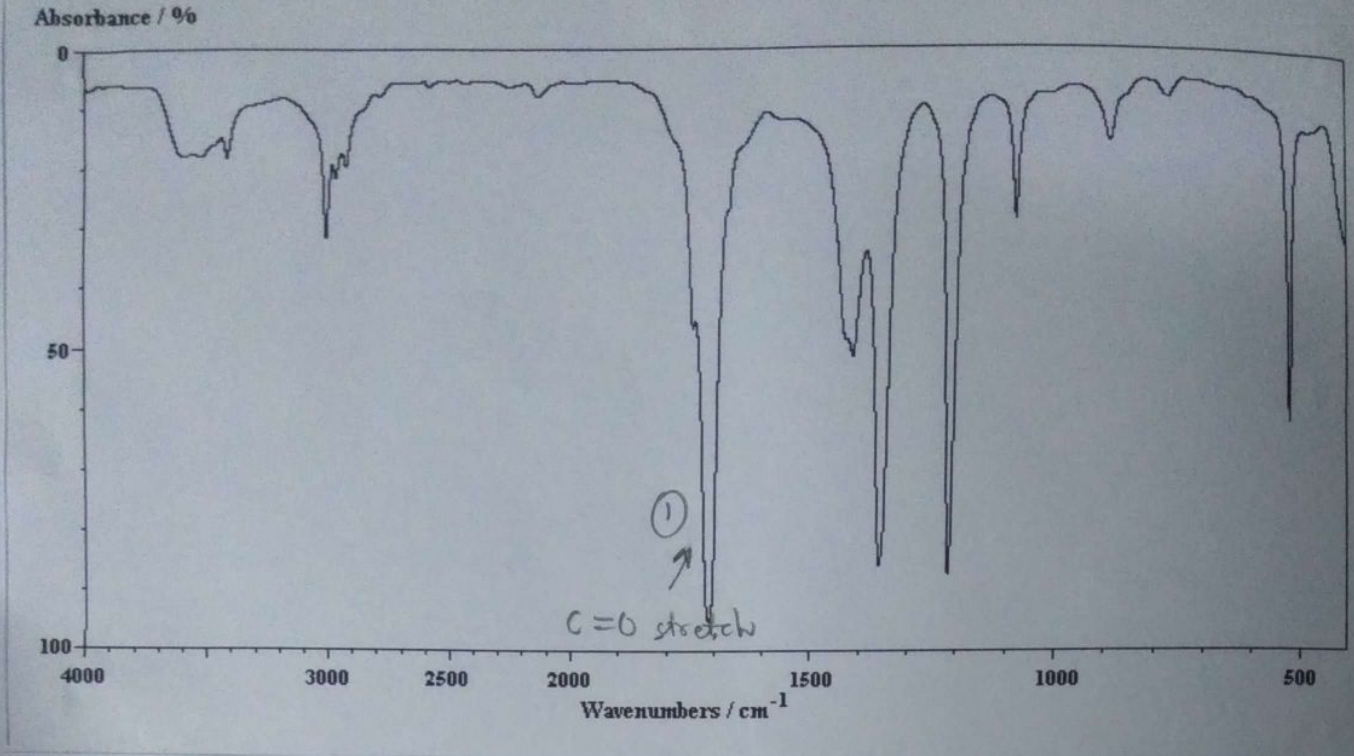
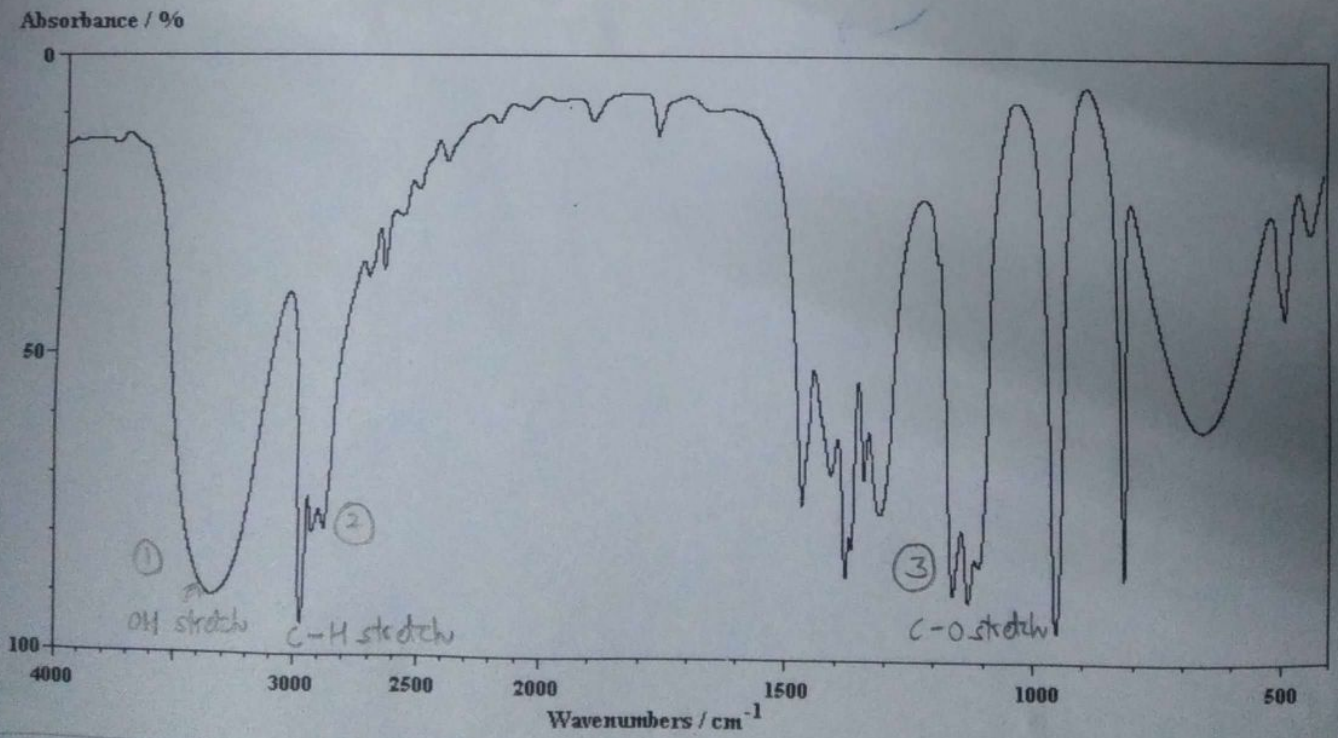


(A) IR spectrum of $H_3C-\overset{\overset{O}{\|}}{C}-CH_3$ (Acetone)



(B) IR spectrum of $CH_3-\overset{\overset{OH}{|}}{\underset{\underset{H}{|}}{C}}-CH_3$ (propan-2-ol)

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In spectrum (B), peak (1) at 3350 - 3200 cm^{-1} corresponds to -OH group (from the table of IR absorptions).

peak (2) corresponds to C-H stretching in 2850-3000 cm^{-1},

peak (3) corresponds to C-O stretching in 1085 - 1050 cm^{-1}.

Thus suggesting that (A) is a ketone & (B) is an alcohol.

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