IR-Spectra Of Cinnamic Acid

EXPT. NO. 4

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19.11.13

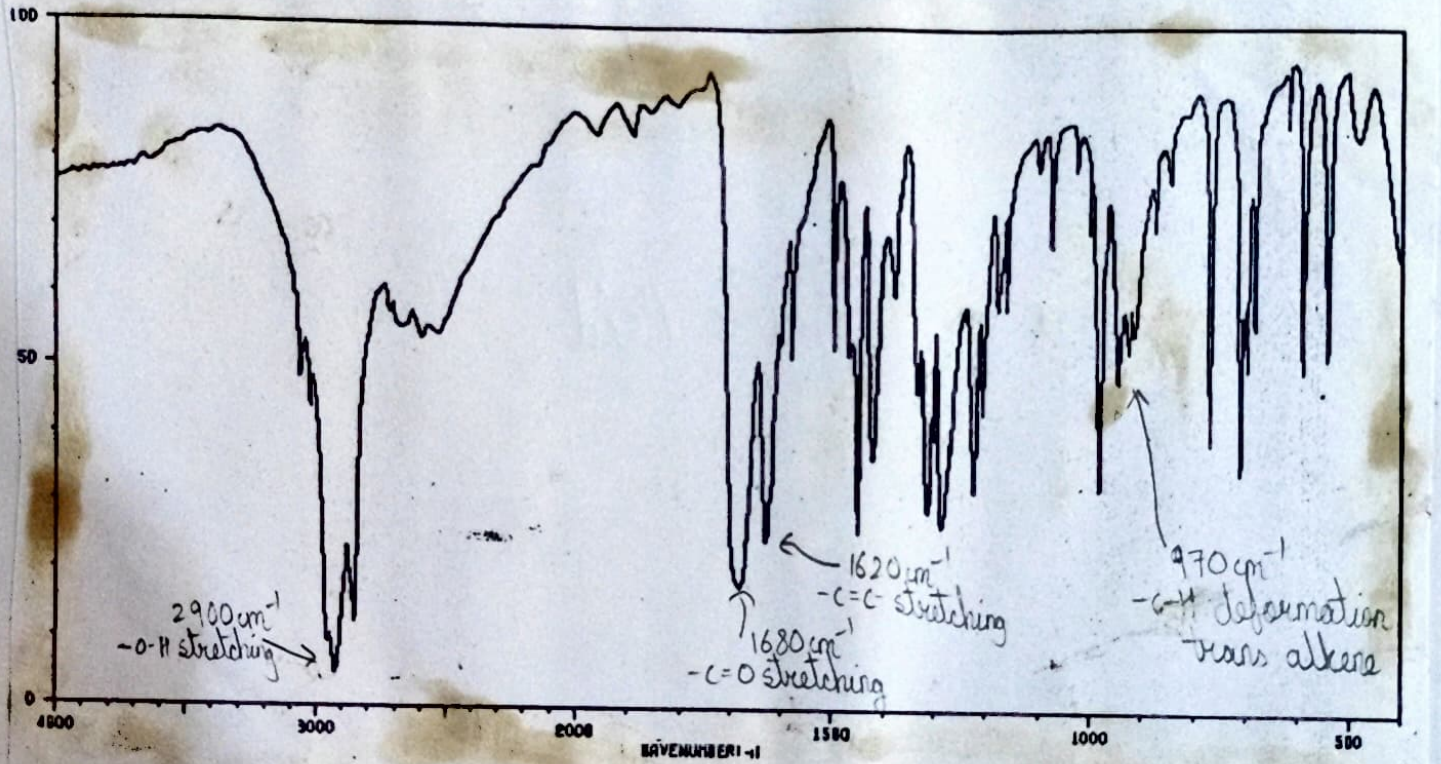
	Stretching Frequency $\bar{\nu}$ in cm^{-1}	Nature	Possible Assignment
(i)	970	medium	trans C-H deformation
(ii)	1620	medium	-C=C stretching
(iii)	1680	strong	-C=O stretching
(iv)	2900	strong	-O-H stretching

Explanation: A broad spectra is obtained in between 2500-3100 which indicates that there is a intramolecular H-bonding and on dilution the absorption peak doesnot change.

(ii) -C=O appears at 1680 cm^{-1}. This is the lower absorption frequency due to the +R effect of phenyl group and C=C bond get single and also -C=O bond, so there is extensive conjugation occurs so peak frequency decrease.

(iii) The frequency at 1620 cm^{-1} indicates the >C=C<

(iv) -C-H deformation band appears at 970 cm^{-1} indicates that the compound is trans.


100
50
0
4000
3000
2000
1500
1000
500
WAVENUMBERI -cI
2900 cm⁻¹
-O-H stretching
1680 cm⁻¹
-C=O stretching
1620 cm⁻¹
-C=C- stretching
970 cm⁻¹
-C-H deformation
-trans alkene

^1H-NMR Of Cinnamic Acid

EXPT. NO.

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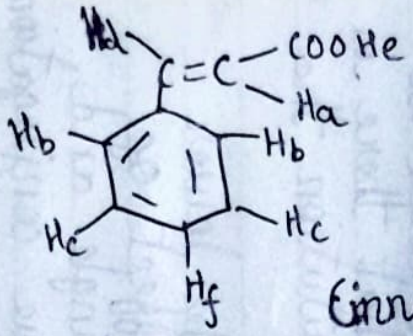
	Chemical Shift δ in ppm	Relative ratio of Protons	Splitting Pattern	Probable Assignment
(i)	6.45	1	doublet	Ha (H of =CHCOOH)
(ii)	7.42	2	doublet	Hb (Ar H)
(iii)	7.56	2	multiplate	Hc (Ar H)
(iv)	7.8	1	doublet	Hd (H of C=C)
(v)	12.7	1	singlet (broad)	He (H of -COOH)
(vi)	7.42	1	triplet	Hf (H of Ar-H)

Explanation: There are five signals observed

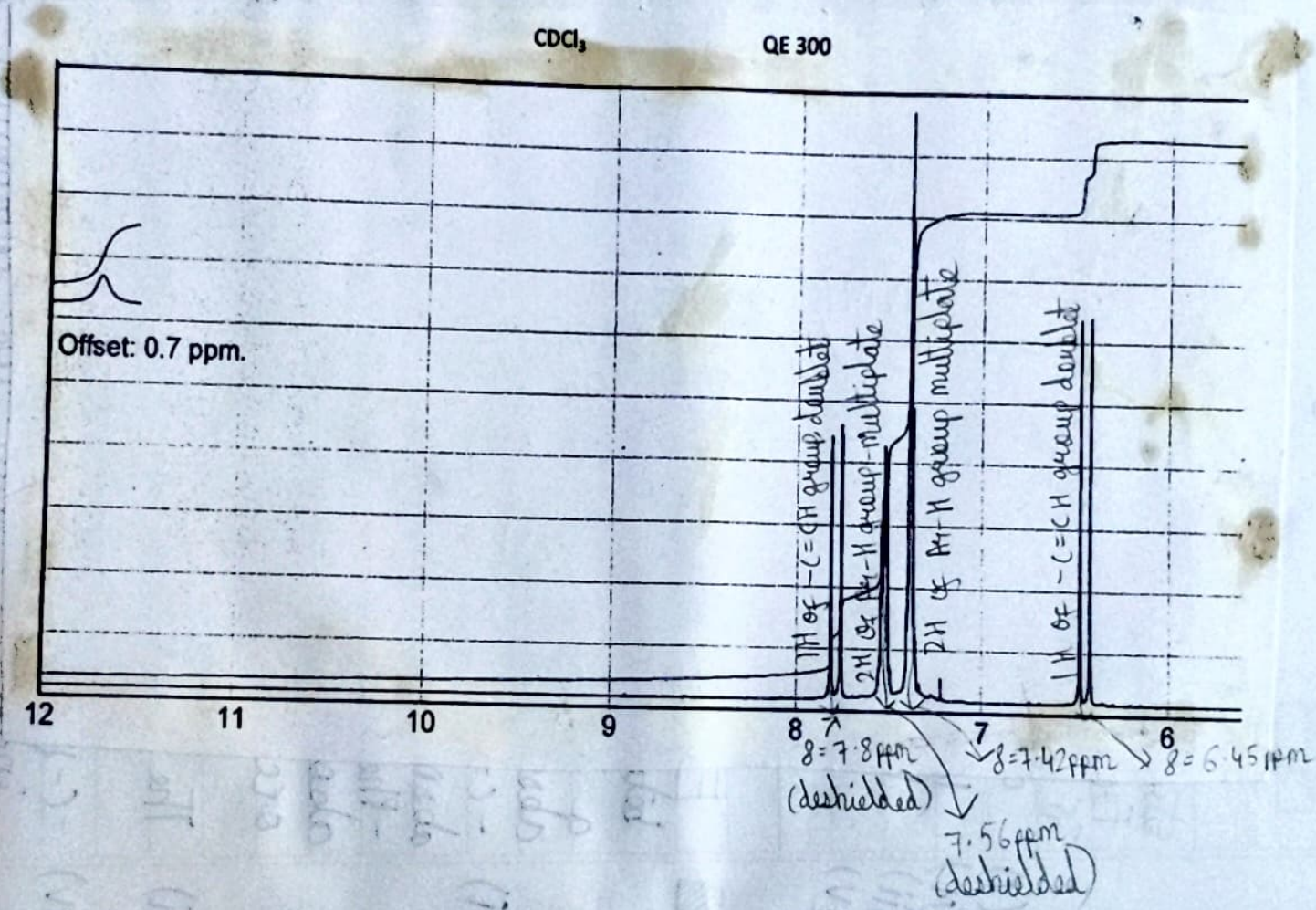
Ha: H of =CHCOOH $\delta = 6.45$ ppm
Hb and Hf: H of ortho and Para of C=CHCOOH group $\delta = 7.42$ ppm
Hd: H of >C=C< $\delta = 7.8$ ppm
He: H of -COOH group $\delta = 12.7$ ppm

(ii) Shielding and Deshielding Effect:

Ha: It experiencing the anisotropic effect of >C=C< and also the -I effect of -COOH so it is deshielded.



Cinnamic Acid



IR-Spectra Of Mesityl Oxide

EXPT. NO. 13

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	Stretching Frequency $\bar{\nu}$ in cm^{-1}	Nature	Possible Assignment
(i)	2900	medium	SP^3 -C-H stretching
(ii)	1700	strong	-C=O stretching
(iii)	1640	strong	-C=C- stretching
(iv)	1450, 1360	medium	$-C-Me_2$ stretching

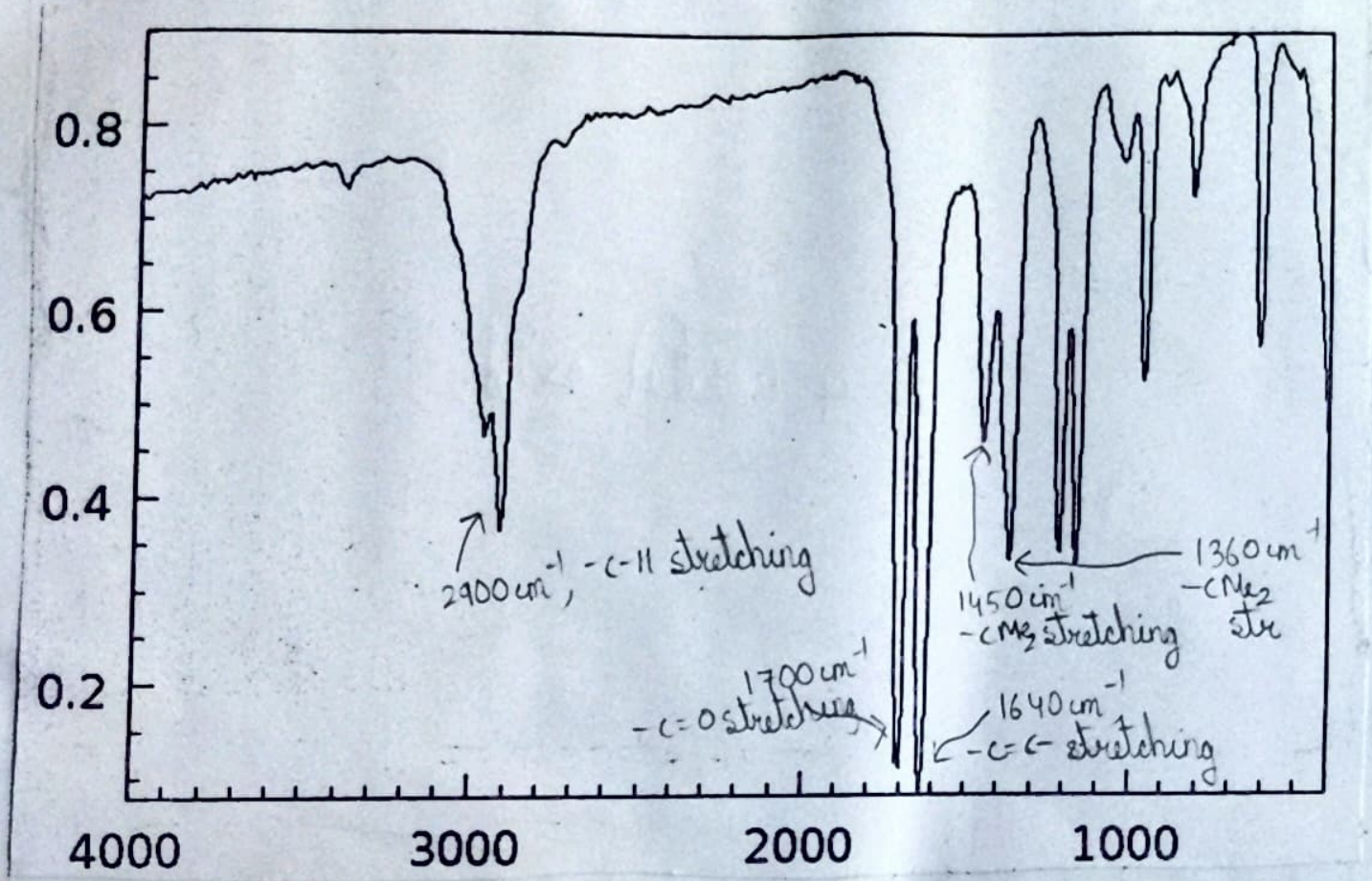
Explanation:

(i) SP^3 -C-H stretching appears at 2900 cm^{-1}

(ii) -C=O appears at the 1700 cm^{-1} because of conjugation took place in between -C=C and -C=O so lower will be the absorption peak.

(iii) A strong band appears at 1640 cm^{-1} indicates -C=C- stretching.

(iv) Two absorption peaks appear at 1450 cm^{-1} and 1360 cm^{-1} due to the symmetric and assymetric stretching of $-CMe_2$.


0.8
0.6
0.4
0.2
4000
3000
2000
1000
2900 cm⁻¹, -C-H stretching
1700 cm⁻¹
-C=O stretching
1450 cm⁻¹
-CH₂ stretching
1360 cm⁻¹
-CH₂ str
1640 cm⁻¹
-C=C- stretching

^1H-NMR Spectra Of Mesityl Oxide

EXPT. NO.

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	Chemical Shift (δ in ppm)	Relative ratio of protons	Splitting Pattern	Probable Assignment
(i)	6.08	1	singlet	Ha (H of >C=C<)
(ii)	2.16	3	singlet	Hb (H of $-COCH_3$ group)
(iii)	2.12	3	singlet	Hc (H of $-CH_3$ group)
(iv)	1.91	3	singlet	Hd (H of $-CH_3$ group)

Explanation:

(i) **Signal Number:** There are four signals for four non-equivalent protons.

Ha : H attached to $-C=C-$ $\delta = 6.1$ ppm

Hb : H of $-COCH_3$ $\delta = 2.15$ ppm

Hc : H of $-CH_3(CMe_2)$ $\delta = 2.12$ ppm

Hd : H of $-CH_3$ $\delta = 1.91$ ppm

(ii) **Shielding and Deshielding Effect:**

Ha : Ha is the most deshielded due to the anisotropic effect of $-C=C-$ and also the electron withdrawing effect of $>C=O$ group.

Hb : Hb is deshielded due to the $-I$ effect of $-C-$ only.

Mesityl oxide