Vibrational studies of Bio molecule: 5-Fluorouracil

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Abstract

FTIR and Raman spectra of uracil & 5-fluorouracil were recorded in the region 200-4000cm^{-1}. Assuming under the C_s point group, the distribution of the normal mode of vibrations between the two species as planar (a') and non-planar (a") are given by 21a'+9a", of which also correspond to the 30 modes of uracil moiety and the electro negativity of fluoro-group substitution causes some mixing/shifting in modes with other modes. The ring breathing and kekule stretching modes are observed to lower magnitudes compared to those for uracil which could be due to mass effect of fluorine atom in place of the hydrogen atom.

Keywords: Infrared spectrum; Raman spectrum; vibrational assignment.

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1. INTRODUCTION

Vibrational studies on 5-fluorouracil and uracil derivatives are used in anti-carcinogenic drugs synthesis against cancer and anti-HIV viruses. 5-fluorouracil is one of the most often used drugs to treat solid tumors and colorectal carcinoma [57]. These molecules do not occur freely in natural biological metabolism. The understanding of the vibrational spectra of the free molecules might be helpful in understanding of specific biological processes and in the analysis of relatively complex systems. Vibrational studies on uracil and its derivatives have been made by several authors [1-29, 48-55, 58-71] although these are still disagreement amongst various works for the assignment modes of uracil. The present article is a part of vibrational spectroscopic study of 5-fluorouracil and deals with the Raman and IR spectra and vibrational assignments for all the 30 normal modes of vibrations.

2. EXPERIMENTAL

Uracil & 5-fluorouracil were purchased from the Aldrich chemical Co. (USA) and were used as such for spectroscopic. All the spectra were recorded at room temperature. The Raman spectra (fig.1-a & b) of the polycrystalline samples were recorded on a Spex-1877 Raman spectrophotometer in the range 200-4000 cm^{-1} using 4880 A^0 line from an C_w Ar^+ laser as the source of excitation, a 2cm^{-1} spectral slit width, a constant scan speed of 0.1 cm^{-1}/sec. and a power less than 100 mw at sample to avoid decomposition of the samples. Infrared spectrum (fig.2-a & b) of samples were recorded in the range 400-4000 cm^{-1} on a Fourier Transform Infra Red (FTIR) spectrophotometer Model-5300 in nujol. The accuracy of the measurement was within ± 3 cm^{-1} and the resolution was better than 2 cm^{-1} for the IR and Raman spectra.

3. RESULTS AND DISCUSSION

The frequencies have been observed in the IR and Raman spectra along with their relative intensities and proposed vibrational assignment of the fundamental modes are given in Table 1. Table 2 contains assignment for the lattice modes, overtones and combination bands. The parent molecule uracil is known to have a planar structure both form the theoretical [35] and experimental [36] studies in the solid phase. Therefore, to a first approximation this molecule may be assumed to belong to the C_s point group. Under the C_s point group the distribution of the normal modes between the two species are given by 21a’+9a”, of which 30 modes also correspond to the uracil moiety. All of the modes are allowed to appear both in the Raman and in the IR spectra.

The complexity of the spectra of the nucleic acid bases makes vibrational assignments rather difficult. Susi et al. [11, 12, 41] have observed that skeletal mode of uracil appear to be surprisingly close and therefore, one might expect a similar pattern for the skeletal modes of the 5-fluorouracil. In the assignment of 5-fluorouracil modes, assistance has also been taken from studies on uracil and substituted uracils [1-29, 38, 39, 43, 46, 48-55, 58-71]. The assignment of the normal modes of 5-fluorouracil may be discussed under the following sections:

NH/ CH modes, C-F modes, C=O modes and pyrimidine ring modes.

3.1 *NH/CH modes*

The NH and CH stretching modes usually appear in the region 3000-3200 cm^{-1} with the N_1H, N_3H and C_6H stretching modes on higher frequencies site are in accordance with the reported works [1, 4, 24, 32, 39, 45]. The Raman/IR spectra show two strong band peaks at 3185/3180 and 3160/3165 cm^{-1} for N_1H and N_3H stretching modes, also one C_6H stretching modes appears with medium strong peak band at3060/3065 cm $^{-1}$ in given table1. The N_1H, N_3H and C_6H in plane bending deformations are observed at 1510/1515, 1420/1410 and 1185/1180 cm $^{-1}$ in accordance with [1, 2, 39, 44].

In uracil and 5-fluorouracil, the out-of-plane NH bending have been assigned in the region 800-860 cm^{-1} [18, 38, 39] and I assign the frequencies 820/835 and 875/880 cm^{-1} to the $\gamma(N_1H)$ and $\gamma(N_3H)$ modes respectively. One out-of-plane C_6H bending in all is assigned at 955 cm $^{-1}$ as in [44] and similar to the 2-thiouracil [1].

3.2 *C-F modes*

In aryl halides(halogen substituted aromatics benzene ring) there are no bands obviously comparable to the aliphatic C-F stretching bands due to interaction with ring vibration .One ring vibration which is mass sensitive and involves some C-F stretching is found approximately at 1300-1100 cm $^{-1}$ [56]. In benzene derivatives containing CF_3 group frequency around 1340 cm^{-1} is observed in IR and Raman spectra which appear to be a characteristic frequency of CF_3 group [4, 28, 29, 31-34]. In a parallel study of the vibrational spectra of 5-substituted uracils with substituent as 5-X-uracil (X=F, Cl, Br, I, NH_2 and CH_3), the C-CH_3 stretching mode and C-NH_2 stretching mode are expected to appear at markedly higher frequencies than in aromatic amines. For 5-aminouracil and 5-methyluracil I have assigned the frequency respectively 1365 cm^{-1} and 1360 cm^{-1} to this mode in agreement with the assignment of trifluoromethyl anilines [40] and cytosine [41]. In the present case, from the comparative study of 5-Fluorouracil, the IR and Raman line have been correlated both at 1350 cm^{-1}. In β(C-NH_2) and γ(C-NH_2) modes for the 5-amonouracil and β(C-CH_3) and γ(C-CH_3) modes for the 5-methyluracil are observed with strong band peaks at 230 and 205 cm^{-1} which is closely agreed with assignment of [40] and also nearly associated with the in-plane bending and out-of-plane bending frequencies for 2-thiocytosine [2] at very strong IR band peaks. In the present case of 5-fluorouracil, the β(C-F) and γ(C-F) modes are observed with strong band peaks at 205 and 175 cm^{-1}.

3.3 *C=O modes*

The most interesting modes of uracil and 5-fluorouracil have an out of the six C=O modes as: the two stretching modes- ν (C_4=O_8) & ν (C_2=O_7), two in-plane bending modes- β (C_2=O_7) and β (C_4=O_8) and two out-of-plane modes- γ (C_2=O_7) and γ (C_4=O_8). The two stretching modes ν (C_4=O_8) & ν (C_2=O_7) are easily identified as strong and IR/ Raman band peaks at 1690/1680 & 1735 for uracil and 1700/1695 & 1735 /1730 cm^{-1} for 5-Fluorouracil respectively, obviously it has also been assigned by authors [1, 4, 15, 20, 21]. Out of the two ν (C=O) modes, the mode due to ν (C_4=O_8) is assigned at lower magnitude as the oxygen atom attached to the C_4 atom participates in the hydrogen bonding due to intermolecular forces which weaken the C_4=O_8 band thereby reduces the magnitude of the ν (C_4=O_8) mode in uracil molecule but in case of 5-Fluorouracil, the fluorine atom being a most electronegative is expected to withdraw electronic charge of C_4 atom resulting a slight positive charge on it . This would effectively shorten the C_4=O_8 bond–length and increase the magnitude of ν (C_4=O_8) mode than the mode of uracil is a most interesting feature of the assignment.

The two C=O deformation modes have some controversies in the assignment are expected to in the region 300-900 cm^{-1}. These two modes β (C_2=O_7) and β (C_4=O_8) in-plane bending modes are observed in IR/ Raman strong band peaks at 560/570 and 550/540 cm^{-1}. But however, some workers for these two C=O in-plane bending modes have been assigned near at ~390 and ~625 cm^{-1} by [15, 18, 37, 41] for uracil and its derivatives. These bands having similar characteristic are also observed in the both IR and Raman spectra of 5-Fluorouracil. The γ (C=O) modes have been proposed near 430 cm^{-1} by some workers [15, 18]. Whereas some other workers [24, 39, 44, 49] have proposed in region 680-820 cm^{-1} for these modes and I agree with the assignments of the latter group of workers. For the uracil and 5-Fluorouracil these bands are observed with very strong peaks at 785/790 and 770 cm^{-1} and have been correlated to the two γ (C_2=O_7) and γ (C_4=O_8) modes. The participation of the O_8 atom in intermolecular hydrogen bonding is expected to the make the planar as well as the non-planar C_4=O_8 motion is more difficult compared to the corresponding modes due to the non-bonded one (C_2=O_7 motion). Hence, the planar and non-planar bending modes due to the C_4=O_8 bond are expected to have lower magnitude compared to that due to the C_2=O_7 bond in accordance with [4, 44].

3.4 *Pyrimidine ring*

The pyrimidine ring similar to the phenyl ring has 12 normal modes of vibration six of which correspond to the ring stretching (ν), three to the ring in-plane deformation (α) and three to the ring out-of-plane deformation (δ) modes. The stretching modes of pyrimidine ring are complicated combinations of the stretching of the C-N, C=N, C-C and C=C bonds of the ring. The ring stretching modes have been observed and correlated to the frequencies 1655/1650, 1450/1455, 1325/1335, 1250/1235 (as kekule mode),1010 /1000 and 760/745 cm^{-1} (as ring breathing) for uracil and 5-Fluorouracil respectively. These assignments are good agreement with those proposed for uracil [49] and its derivatives [1, 2, 4, 38, 44]. However, it is difficult to assign the ring breathing and kekule stretching modes due to complexity owing to the mixing of the ring stretching (C-N, C=N, C-C and C=C bonds of the ring) with other modes. The ring breathing and kekule modes in the present case which are also lower in magnitudes compared to their counter parts of the phenyl rings. The frequency 1250 cm^{-1} for uracil and 1235 cm^{-1} for 5-Fluorouracils are comparatively lower in magnitudes than the parent molecule uracil due to mass of substituted halogen atom with strong peak could be correlated to the Kekule type vibration mode (ν_{14}) of benzene whereas type frequency 760 cm^{-1} for uracil and 745 cm^{-1} for 5-Fluorouracil in a lower magnitudes than the parent molecule uracil due to mass of substituted halogen atoms, showing the similar to the that of ν_1 of benzene is identified as the ring breathing vibration of the pyrimidine ring as similar to [44].

Similar to benzene and its derivatives[30-34, 40, 42, 47], out of the three in-plane ring deformation or angle bending modes, the mode due to trigonal angle ring bending is one of the interesting and most widely discussed mode as similar to the ring breathing and Kekule ring modes. The frequency of this mode is substantially reduced due to its strong mixing with other modes. The planar ring deformation are assigned at 982, 559/536 and 516 cm^{-1} by has Harsanyi et al. [49], at 802, 548 and 480 cm^{-1} by Colombo and Kirin [39], at 785, 556 and 482 cm^{-1} by Susi and Ard [12], at 995, 732 and 480 cm^{-1} by Szczesniak et al. [23] & for 5-trifluoromethyl uracil at 1009, 637 and 446 cm^{-1} [4]. In the present case the frequencies 995/980, 670 /665/655 and 445/455 cm^{-1} are assigned to the plane ring deformation with a good agreement to the reported workers [4, 8, 23, 44, 49]. The three ring torsional or out-of-plane deformation modes, in 1-methyluracil [39] of these modes have been proposed at 525, 445, and 268 cm^{-1} and for 5-trifluoromethyl uracil at 602, 418, and 208 cm^{-1} by Yadav et al. [4] are a good agreement with uracil and 5-Fluorouracil of the ring torsional modes frequencies at 630, 415/420 and 260 cm^{-1} close with [44].

4. CONCLUSIONS

All the 30 normal fundamental modes of uracil and 5-Fluorouracil could be assigned in the present case. The ring breathing, Kekule and trigonal angle bending modes are observed to have closely same magnitudes with 5-trifluoromethyl uracil. The ring breathing and kekule stretching modes are observed to lower magnitudes compared to those for uracil which could be due to mass effect of fluorine atom in place of the hydrogen atom and the electro negativity of fluorine group substitution causes some shifting in the ν (C_4=O_8) mode than the mode of the parent molecule uracil.

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Table1.Fundamental frequencies* of uracil & 5-fluorouracil

Infrared(IR) (cm^{-1})		**Raman (cm^{-1})**		**Assignments$^\$$**
Fig.2		**Fig.1**		
(a)	**(b)**	**(a)**	**(b)**	
U	5-F-U	U	5-F-U	
3180(m)	3185(m)	----	3185(vs)	a’ $\nu(N_1H)$
3160(m)	3165(m)	----	3160(vs)	a’ $\nu(N_3H)$
3095(m)	nil	3100(w)	nil	a’ $\nu(C_5H)$
3060(m)	3065(m)	3065(s)	----	a’ $\nu(C_6H)$
1735(vs)	1735(s)	1735(m)	1730(s)	a’ $\nu(C_2{=}O_7)$
1690(vs)	1700(vs)	1680vs)	1695(vs)	a’ $\nu(C_4{=}O_8)$
1650(vs)	1650(vs)	1655(ms)	1655(ms)	a’ $\nu(C_5{=}C_6)$ring
1510(m)	1505(m)	1510(ms)	1515(m)	a’ $\beta(N_1H)$
1450(s)	1450(vs)	1455(s)	1455(w)	a’ ν (ring)
1410(vs)	-----	1410(vs)	1420(s)	a’ $\beta(N_3H)$
nil	1350(ms)	nil	1350(vs)	a’ $\nu(C_5\text{-}F)$
1320(w)	1320(w)	1335(s)	1325(m)	a’ ν (ring)
1240(vs)	1235(vs)	1250(vs)	1235(vs)	a’ ν (ring)Kekule
1185(m)	1180(m)	1180(m)	1185(m)	a’ $\beta(C_6H)$
1060(ms)	nil	1050(m)	nil	a’ $\beta(C_5H)$
1010(vs)	1000(ms)	1000(s)	1010(s)	a’ ν (ring)
995(vs)	980(m)	995(s)	----	a’ α (ring)
----	955 (m)	----	-----	a” $\gamma(C_6H)$
875(vs)	875(s)	880(s)	875(s)	a” $\gamma(N_3H)$
820 (s)	815 (vs)	835(ms)	820(ms)	a” $\gamma(N_1H)$
805(sh)	nil	805(ms)	nil	a” $\gamma(C_5H)$
790(sh)	-------	790(s)	785(vs)	a” $\gamma(C_2{=}O_7)$
770(s)	-------	----	----	a” $\gamma(C_4{=}O_8)$
760(s)	745(s)	----	----	a’ν(ring)breathing
670(w)	665(s)	655(m)	655(vs)	a’ α (ring)
630(w)	----	610(w)	----	a” δ (ring)
570(m)	----	560 (m)	560 (vs)	a’ $\beta(C_2{=}O_7)$
540(m)	550(vs)	540(m)	----	a’ $\beta(C_4{=}O_8)$
440(vs)	448(vs)	450(m)	455(vs)	a’ α (ring)
----	420(s)	415(w)	415(vs)	a” δ (ring)

			260(s)	----		a” δ (ring)
			nil	205(m)		a’ β (C_5 -F)
			-nil	175(vs)		a” γ(C_5 -F)

[*]vw = very weak, w = weak, m = medium, mw = medium weak, ms =medium-strong, s =strong, vs = very strong, sh = shoulder, ssh =strong shoulder. [$]ν: stretching, α: angle bending, β: in-plane bending, γ =out-of-plane bending, δ = out-of-plane ring deformation or ring torsion.

Table2. Lattice modes, overtones and combination frequencies* of uracil & 5-fluorouracil

Infrared(IR) (cm^{-1})			Raman (cm^{-1})			Assignments[$]
Fig.2			Fig.1			
(a)	(b)		(a)	(b)		
U	5-F-U		U	5-F-U		
3210(m)						1705+1505
						1655+1455
			2935(m)			1915+1420
2920(m)	2920(s)					1510+1410
	2900(s)			2900(s)		1450x2(ring)
2820(m)	2825(s)			2825(m)		1410x2
	1875(m)					1000+875
1830(w)	1830(m)		1830(m)			1010+820
1785(s)						1010+875
1620(m)			1615(s)			995+625/620
			1120(m)			560x2
						545x2
						620+445
						630+260
						420+260
						420+205
						260+205
						Intermolecular/lattice
						Intermolecular/lattice
						Intermolecular/lattice
						Intermolecular/lattice

[*]Abbreviations are similar to those defined in Table 1.

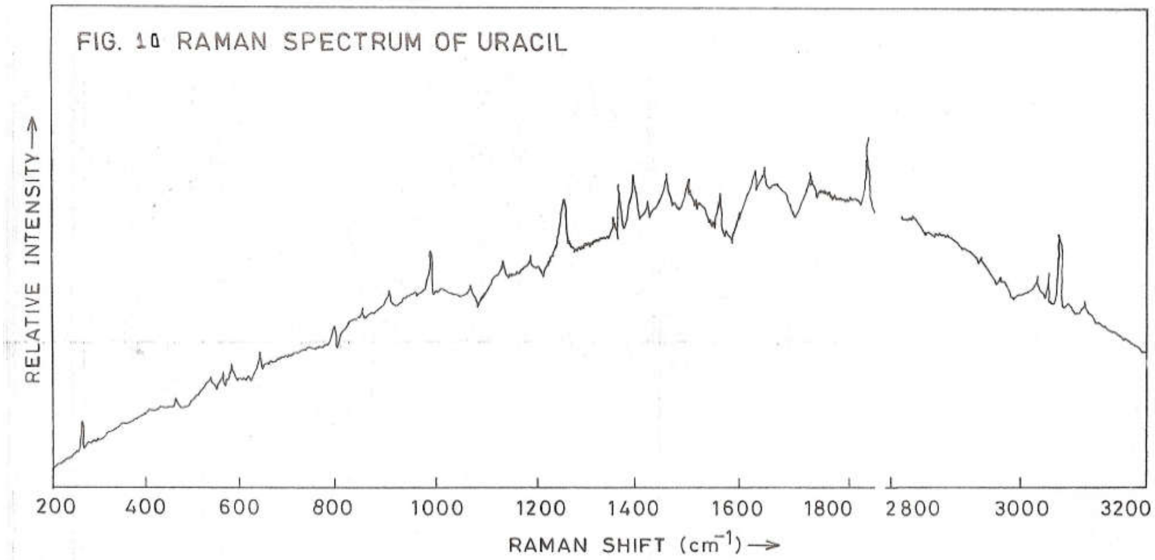

FIG. 1a RAMAN SPECTRUM OF URACIL

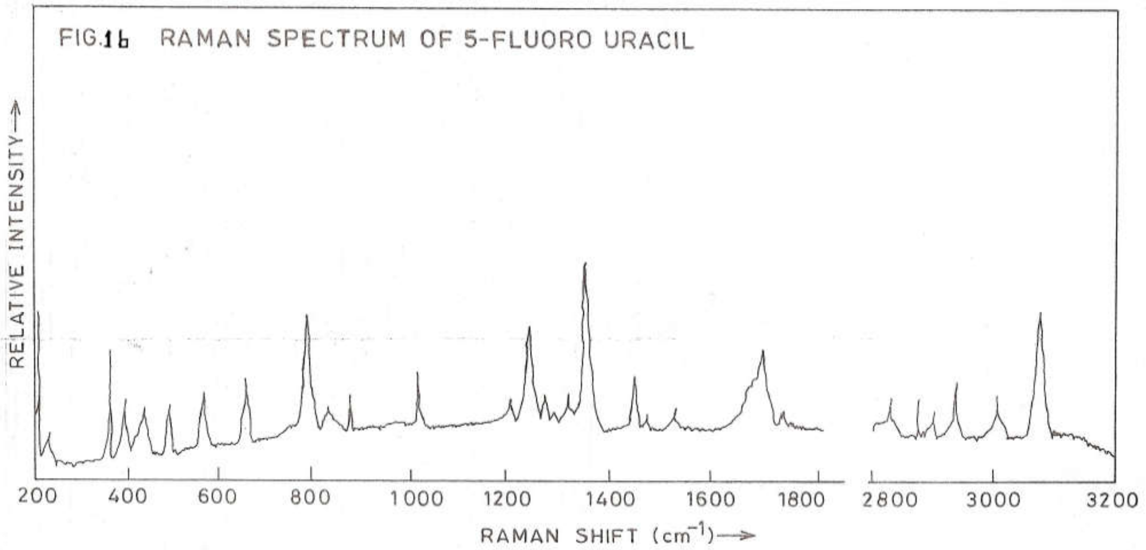

FIG.1b RAMAN SPECTRUM OF 5-FLUORO URACIL

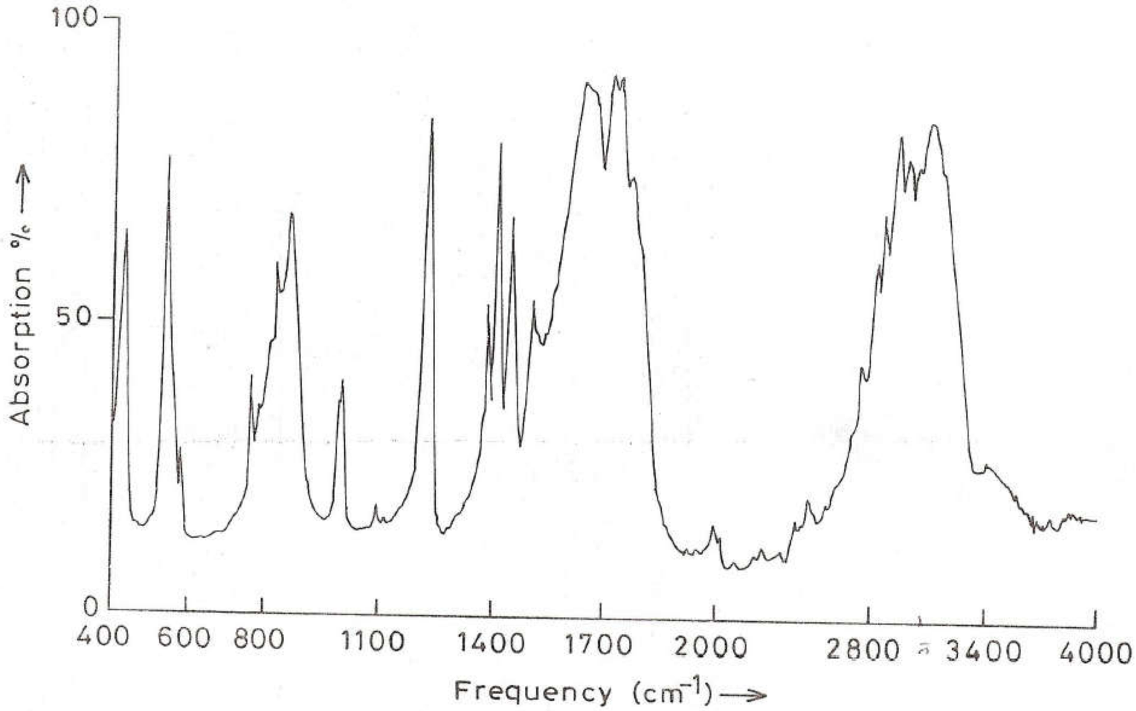

FIG.2a INFRARED SPECTRUM OF URACIL (IN NUJOL)

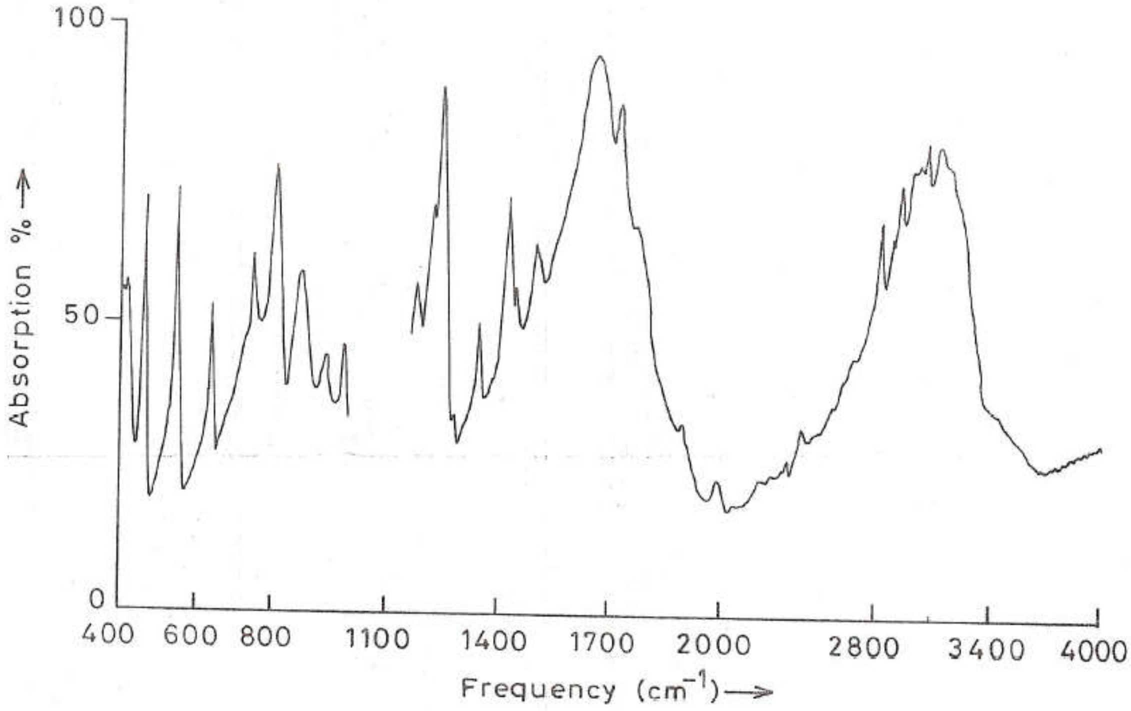

FIG.2 b INFRARED SPECTRUM OF 5-FLUORO URACIL (IN NUJOL)