Laser Raman and IR Spectra of Biomolecule:
5-Methyluracil (Thymine)

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ABSTRACT

Raman (200-$4000cm^{-1}$) and IR (400-$4000cm^{-1}$) spectra of 5-methyluracil (thymine) have been recorded and analysed in the region 200-$4000cm^{-1}$ and vibrational assignment for all the 39 (26a' + 13a") normal modes are proposed and distributed as 26a' species of planar and 13a" species of non-planar vibrations. Consistent assignments have been made for the internal modes of the CH_3 group, especially for the anti-symmetric CH_3 stretching and bending modes. However, assuming 5-methyluracil to be non-planar molecule, splitting of all the frequencies could be very well explained. A possible explanation could be the planarity of the pyrimidine ring and non-planarity at carbon site of the methyl group which might cause splitting of the frequencies including three components. The non-equivalence of the three CH bonds of the CH_3 group suggests a difference in the strength of the other CH bond on the pyrimidine ring. These three CH_3 stretching frequencies are distinctly separated from the CH/NH ring stretching frequencies. 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.

Keywords: Infrared spectrum; Raman spectrum; vibrational assignment.

1. INTRODUCTION

The vibrational studies of molecular spectra of the nucleic acid bases and their derivatives are of the considerable importance from biological point of view as these are constituents of the important bio-molecules 5-methyluracil (thymine) for DNA and uracil for RNA as a genetic material and these pyrimidine derivatives are essential ingredients of soluble ribonucleic acid and their derivatives are used in anti-carcinogenic drugs synthesis against cancers and anti-HIV viruses. 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 have been made by several authors [1-29, 49] although these are still disagreement amongst various works for the assignment modes of uracil. We plan to perform a symmetric study of the vibrational spectra of 5-substituted uracil with substituent as CH_3, NH_2, F, Cl, Br and I in the spectroscopic investigation. The present article is a part of vibrational spectroscopic study of 5-X-uracils (X=F, Cl, Br, I, NH_2 and CH_3) for all the normal modes vibration.

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2. EXPERIMENTAL

5-methyluracil was purchased from the Aldrich chemical Co. (USA) and was used as such for spectroscopic. All the spectra were recorded at room temperature. The Raman spectrum (fig.1) of the polycrystalline sample was 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 2 cm^{-1} spectral slit width, a constant scan speed of 0.1 cm^{-1}/sec. and a power less than 100mw at sample to avoid decomposition of the samples. Infrared spectrum (fig.2) of 5-methyluracil powder was recorded in the range 400-4000 cm^{-1} on a Fourier Transform Infra Red (FTIR) spectrophotometer Model-5300 in nujol. IR spectrum (fig.3) was also recorded at room temperature in the range 600-4000 cm^{-1} on a Perkin-Elmer-1320 spectrophotometer in KBr pellet of optics. The accuracy of the measurement was within $\pm$ 3 cm^{-1} and the resolution was better than 2 cm^{-1} for the IR and Raman spectra.

3. RESULTS AND VIBRATIONAL ASSIGNMENTS

The frequencies 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. To the best of our information no structural data are available for 5-methyluracil in literatures. 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 symmetry one of three hydrogen atoms of the CH$_3$ group has to be taken in the plane and the remaining two have to be taken symmetrically below and above the plane of the uracil ring [46]. Under the C$_s$ point group the distribution of the normal modes between the two species are given by 26a'+13a'', of which 30 modes (21a'+9a'') correspond to the uracil moiety and 9 modes (5a'+4a'') to the CH$_3$ group. 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. H. 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-methyluracil. In the assignment of 5-methyluacil modes, assistance has also been taken from studies on uracil [1-27], CH$_3$/CF$_3$ group containing benzene derivatives [40, 50, 51] and substituted uracil [1, 38, 39]. The assignment of the normal modes of 5-methyluracil may be discussed under the following sections:

3.1   CH$_3$ modes, 3.2 NH/ CH modes, 3.3 C-CH$_3$ modes, 3.4 C=0 modes and 3.5 pyrimidine ring modes.

3.1 *CH$_3$ modes*

The CH$_3$ group give rise to 9 internal modes of vibrations, namely as: 1-symmetric stretching- ν_s (CH$_3$), 2-anti-symmetric stretching- ν_{as} (CH$_3$), 1-scissoring or symmetric deformation or simply deformation- δ_a (CH$_3$), 2-anti-symmetric deformations - δ_{as} (CH$_3$), 1- parallel rocking to the plane- $\rho_{\parallel}$ (CH$_3$), 1- perpendicular rocking to the plane/wagging- $\rho_{\perp}$ (CH$_3$) and 1-torsion or twist- τ (CH$_3$) modes. Thus the three CH$_3$ stretching modes are observed at three different frequencies. However, assuming thymine to be a non-planar molecule, splitting of all

the frequencies could be very well explained. A possible explanation could be planarity of the pyrimidine ring and non-planarity at the carbon site of the methyl group which might cause splitting of frequencies into three components. Non-equivalence of the three CH bonds of the CH_3 group suggests a difference in the strengths of the other CH bonds of on pyrimidine ring. The two ν_{as} (CH_3) and one ν_s (CH_3) modes appear in the region 2800-3000 cm^{-1}[51].In the present case, the symmetric CH_3 -ν_s (CH_3) is assigned at 2900 cm^{-1} and is observed to have a strong Raman intensity. The two anti-symmetric CH_3 -ν_{as} (CH_3) of one lower frequency mode has assigned with very strong Raman band at 2925 cm^{-1} for a' species and other higher frequency mode has assigned with strong Raman band at 2998 cm^{-1} for a'' species and respectively for each one modes, IR bands are at 2925 and 3000/3005 cm^{-1}.The Raman line corresponding to the lower frequency appears usually (in benzene derivatives) with higher intensity and the lower depolarization ratio is suggesting its origin due to more symmetric mode. In light of this observation, I associated the lower frequency to the ν_{as} (CH_3) mode under a' species and the other one to that under a'' [4].

The two anti-symmetric and one symmetric CH_3 deformation modes appear in the region 1350-1500 cm^{-1}[52, 53].Out of the three deformation modes, the ν_s (CH_3) appears in both Raman and IR spectra with a very strong intensity at 1375 cm^{-1} could be correlated to the umbrella type vibration mode as good agreement with [52]. The assignment of the two ν_{as} (CH_3) modes are assigned at different frequencies 1465 and 1425 cm^{-1} with good intensity in both Raman and IR spectra as reported by [53] for methyl group frequencies. The above methyl group shows some sensitivity to the electro negativity of the attached atom.

Methyl group rocking frequencies are mass sensitive and variable in position due to interaction with skeletal stretching modes. The two CH_3 rocking modes are expected to appear in the region 1150-1100 cm^{-1} and 900-850 cm^{-1} for perpendicular and parallel rocking modes respectively [54]. In accordance with above, these are assigned at 1155 cm^{-1} for $\rho_\perp$ (CH_3) and 900 cm^{-1} for $\rho_{||}$ (CH_3) modes.

The CH_3 torsional frequency along the C-CH_3 bond has more complexity as shown in the assignments [2, 30, 34, 43, 48]. Due to remove the complexity in τ (CH_3) mode has been done the parallel studies of substituted uracil [5-X-uracil, X= F, Cl, Br I, NH_2 and CH_3] with a comparison of τ (CH_3) mode is clearly expected at 340 cm^{-1} as closed with the assignments [30, 34].

3.2 NH/CH modes

The NH and CH stretching modes usually appear in the region 3000-3200 cm^{-1} with the three N_1H, N_3H and one C_6H stretching modes on higher frequencies site are in accordance with the reported works [1, 4, 24, 32, 39, 45]. The IR band spectrum shows two band peaks at 3185 and 3160 cm^{-1} for N_1H and N_3H stretching modes, also one C_6H stretching modes appears with very strong Raman band at 3065 cm^{-1} in given table 1. The N_1H, N_3H and C_6H in plane bending deformations are observed at 1515, 1420 and 1200 cm^{-1} in accordance with [1, 2, 39] and are given in table 1.

In uracil, the out-of-plane NH bending have been assigned in the region 800-860 cm^{-1} [18, 38, 39] and I assign the frequencies 815 and 850 cm^{-1} to the $\gamma(N_1H)$ and $\gamma(N_3H)$ modes respectively. One out-of-plane C_6H bending is assigned at 940 cm^{-1} and similar to the 2-thiouracil [1].

3.3 C-CH$_3$ modes

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, 47]. The C-CH$_3$ stretching mode is, therefore, expected to appear at markedly higher frequencies than in aromatic amines. In the present case , from the comparative study of 5-X-uracils, the IR and Raman line have been correlated at 1360 and 1355 cm^{-1}. For 5-methyluracil I assign the frequency 1360 cm^{-1} to this mode in agreement with the assignment of [40] and [41]. The 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.

3.4 C=O modes

The most interesting modes of 5-methyl-uracil has all of the six C=O modes, the two C=O stretching modes are easily identified as strong and IR band peaks at 1740 and also in Raman at 1680 cm^{-1}, 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. 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 banding modes are observed in IR strong band peaks at 560, 540 cm^{-1} and in Raman for β ($C_4=O_7$) at 560 cm^{-1} with strong band peak. 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-X-uracils (X=F, Cl, Br, I, CH$_3$ and NH$_2$). The γ (C=O) modes have been proposed near 430 cm^{-1} by some workers [15, 18].Whereas some other workers [24, 39, 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 5-methyl-uracil these bands are observed with very strong peaks at 760 and 745cm^{-1} and have been correlated to the two $\gamma(C_2=O_7)$ 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.

3.5 Pyrimidine ring modes

The pyrimidine ring similar to the phenyl ring has 12 normal modes of vibration six of which correspond to the ring stretching, 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 1645, 1445, 1290, 1240, 1030 and 710 cm^{-1}. These assignments are good agreement with those proposed for uracil [49] and its derivatives [1, 2, 4, 38]. The frequency 1240 cm^{-1} with strong peak could be correlated to the Kekule type vibration mode (v_{14}) of benzene whereas type frequency 710 cm^{-1}, showing the similar to the that of v_1 of benzene with a weak IR band peak, is identified as the ring breathing vibration of the pyrimidine ring.

Similar to benzene and its derivatives, 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 Szczepaniak et at. [23] & for 5-trifluoromethyl uracil at 1009, 637 and 446 cm^{-1} [4]. In the present case the frequencies 995, 640 and 460 cm^{-1} are assigned to the plane ring deformation with a good agreement to the reported workers [4, 8, 23, 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 5-methyluracil of the ring torsional modes frequencies at 610, 420 and 232 cm^{-1} in the given table 1.

4. CONCLUSIONS

For the first time, all the 39 normal fundamental modes of 5-methyluracil could be assigned in the present case. The ring breathing, Kekule and trigonal angle bending modes are observed to have closely same magnitudes for 5-trifluoromethyl uracil, the earlier work [55,56] and the other extensive complete study of derivatives of 5-substituted uracils (5-X-uracils; X=F, Cl, Br, I, NH$_2$ and CH$_3$) on the fifth position of carbon atom (C$_5$) in their pyrimidine rings [57-63]. However, all the C=O modes are observed at nearly same frequencies compared to 5-trifluoromethyl uracil. Symmetry and anti-symmetry CH stretching modes of the CH$_3$ group appear clearly at different frequencies. 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 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. The appearance of all the frequencies could be explained only on the basis of planarity of the pyrimidine ring and non-planarity at the carbon site of the methyl group.

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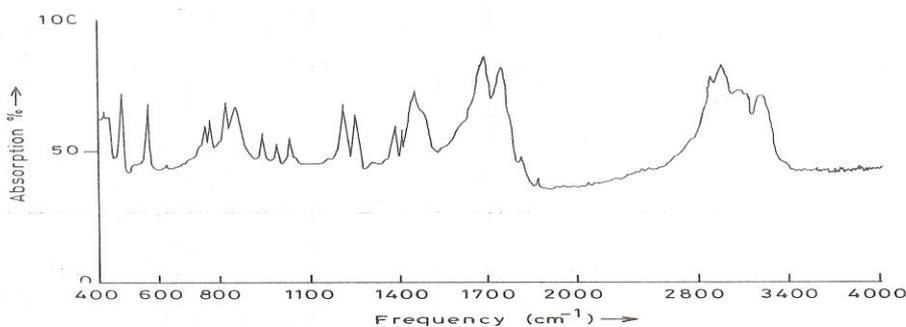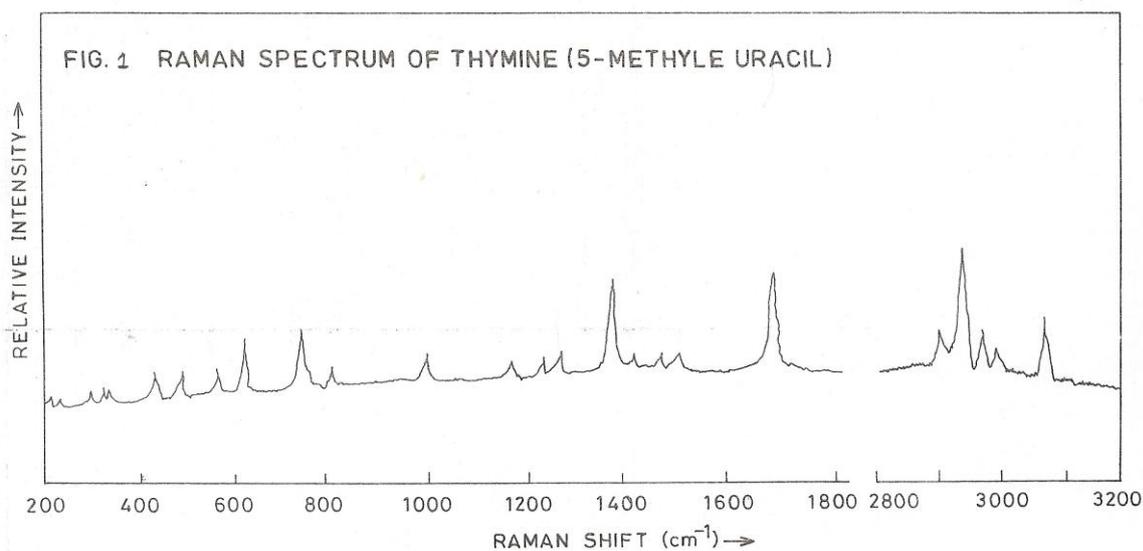[33] R.A. Yadav and I.S. Singh, *Spectrochim. Acta* **41A**, 191 (1985).

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Table1.Fundamental frequencies[*] of 5-methyl-uracil (Thymine)

Infrared cm^{-1}		Raman cm^{-1}	Assignments[$]
Fig.2	Fig.3	Fig.1	
3185(vs)	3185(sh)	----	a' ν (N_1H)
3160(sh)	3160(sh)	----	a' ν (N_3H)
3060(m)	3060(w)	3065 (vs)	a' ν (C_6H)
3005(w)	3000(w)	2998 (s)	a'' ν_{as}(CH_3)
2925 (s)	2925(m)	2925(vs)	a' ν_{as}(CH_3)
2895(sh)	2900(w)	2900 (s)	a' ν_s(CH_3)
1738(vs)	1740 (s)	----	a' ν (C_2=O_7)
1680(vs)	1680(s)	1680(vs)	a' ν (C_4=O_8)
1640(sh)	1645(sh)	-----	a' ν (C_5=C_6) ring
1505(sh)	1505(w)	1515(ms)	a' β (N_1H)
1465(sh)	1465 (s)	1465(ms)	a'' δ_{as} (CH_3)
1445(vs)	1445(vs)	1445(w)	a' ν (ring)
1430(sh)	1430(s)	1425(ms)	a' δ_{as}(CH_3)
1420(s)	1420(s)	----------	a' β (N_3H)
1380 (s)	1375(vs)	1375(vs)	a' δ_s(CH_3) Umbrella
1360(sh)	1360(sh)	-------------	a' ν (C_5–CH_3)
1300(w)	1300(sh)	1290(s)	a' ν (ring)
1240(vs)	1240(vs)	1235 (s)	a' ν (ring) Kekule
1195(vs)	1200(vs)	----	a' β (C_6H)
1145(w)	1150(w)	1155(ms)	a'' $\rho_\perp$ (CH_3)
1030(s)	1030(vs)	-----	a' ν (ring)
985 (s)	995(vs)	995(ms)	a' α (ring)
940 (s)	940(vs)	----	a'' γ (C_6H)
910(w)	900(w)	------	a' $\rho_{\parallel}$ (CH_3)
850(vs)	845(s)	----	a'' γ (N_3H)
815(vs)	815(vs)	815 (ms)	a'' γ (N_1H)
760(s)	760(vs)	-----	a'' γ (C_2=O_7)
745(s)	740(vs)	745(vs)	a'' γ (C_4=O_8)
710(sh)	710(w)	----	a' ν (ring)- breathing
--------	640(w)	640(vs)	a' α (ring)

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610(mw)	610(m)	----	a''	τ (ring)
560(vs)		560 (s)	a'	β ($C_2 = O_7$)
540 (sh)		-----	a'	β ($C_4 = O_8$)
462(vs)		460(s)	a'	α (ring)
420 (s)		420(s)	a''	τ (ring)
		340(ms)	a''	τ (CH_3)
		280(ms)	a''	τ (ring)
		230(ms)	a'	β ($C_5 - CH_3$)
		205(ms)	a''	γ ($C_5 - CH_3$)

[*]vw = very weak, w = weak, m = medium, mw = medium weak, ms =medium-strong, s =strong, vs = very strong, sh = shoulder, ssh =strong shoulder. [$]$\nu$: stretching, s: symmetric, as: anti-symmetric, α: angle bending, β: in-plane bending, γ =out-of-plane bending, δ = deformation, ρ = rocking, τ = torsion/ twist.

FIG. 1   RAMAN SPECTRUM OF THYMINE (5-METHYLE URACIL)

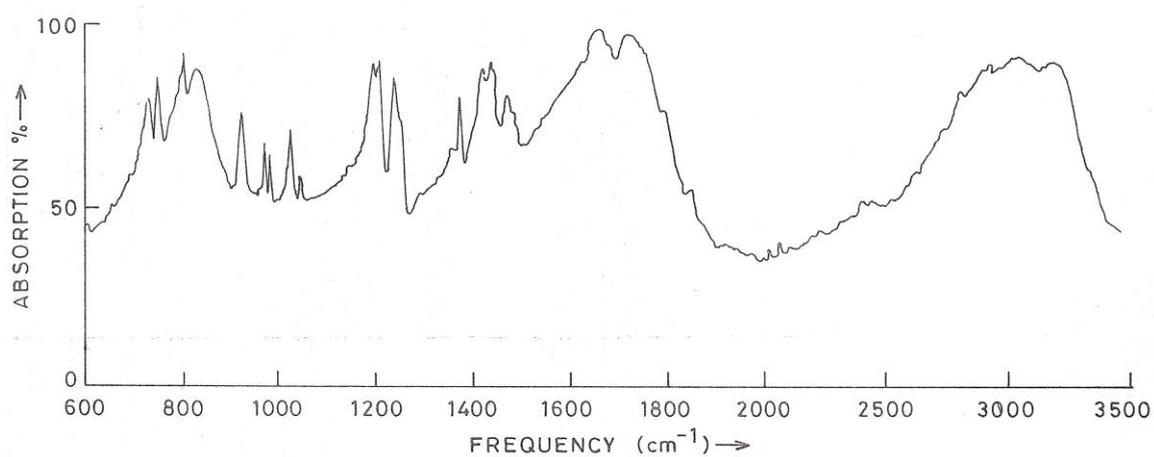FIG. 2   INFRARED SPECTRUM OF THYMINE 5-METHYLE URACIL (IN NUJOL)

FIG.3 INFRARED SPECTRUM OF THYMINE 5-METHYLE URACIL (IN kBr)