FTIR and Raman Spectra Compared with Ab Initio Calculated Frequency Modes for 5-Aminouracil

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Received: 25 February 2008 / Accepted: 2 October 2008 /

Published online: 4 December 2008

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Abstract Infrared (IR) and Raman spectra of 5-aminouracil were recorded in the region 200–4,000 cm^{-1} . Assuming under the C_s point group that the distribution of the normal mode of vibrations between the two species are planar (a') and non-planar (a''), given by $25a' + 11a''$ of which 30 modes ($21a' + 9a''$) correspond to the uracil moiety and six modes ($4a' + 2a''$) correspond to the NH_2 group, with a comparison of theoretically ab initio calculated frequencies, the results are in reasonably good agreement with the experimental IR and Raman spectra. Consistent assignments have been made for the internal modes of the NH_2 group, especially for the anti-symmetric NH_2 stretching and bending modes. The non-equivalence of the two NH bonds of the NH_2 group suggests a difference in the strength of the two hydrogen bonds on the pyrimidine ring. Symmetry and anti-symmetry NH stretching modes of the NH_2 group show the invalidity of the empirical relationship. These two NH_2 stretching frequencies are distinctly separated from the CH/NH ring stretching frequencies. A strong and sharp IR band that acts at 3,380 cm^{-1} could be identified as the anti-symmetric NH_2 mode whereas the band at 3,290 cm^{-1} smaller density could be identified as the symmetric NH_2 stretching mode.

Keywords Infrared spectrum • Raman spectrum • Vibrational assignment

1 Introduction

Vibrational studies on nucleic acid bases and their derivatives are of the considerable importance from a biological point of view as these are constituents of genetic material, for instance, uracil derivatives are used in anti-carcinogenic drug synthesis and anti-HIV drugs.

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These molecules do not occur freely in natural biological metabolism. The understanding of the vibrational spectra of free molecules might be helpful in the understanding of specific biological processes and in the analysis of relatively complex systems. 5-Aminouracil is an analogue of thymine and uracil, nucleobases found in DNA and RNA, respectively. Nucleic acids are polymers of nucleotide. In these polymers, it is well known that the bases from one chain interact with those in the complementary chain to form specific hydrogen bonds between pyrimidine and purine bases, cytosine usually pairing with guanine (GC) and thymine (in DNA) or uracil (in RNA) with adenine (AT or AU). The sequence and specificity of pairing is responsible for the genetic code and ability of DNA to replicate itself accurately for the next generation. The study of the structure and spectra of DNA bases and their derivatives are quite important. Among the different DNA bases, guanine and adenine are the most crucial ones since they are the centers of several biological activities. The photochemistry of thymine is significant; UV-induced photoproducts of thymine in DNA lead to skin cancer and other diseases [1]. 5-Fluorouracil is a derivative of uracil and one of the most often used drugs to treat solid tumours and colorectal carcinoma [2].

Vibrational studies on uracil and its derivatives have been made by several authors [3–44] although there is still disagreement amongst various works for the assignment modes of uracil. I plan to perform a parallel study on the vibrational spectra of 5-substituted uracil with substituent as 5-X-uracils ($X = \text{F, Cl, Br, I, NH}_2 \text{ and CH}_3$). The present article is a part of vibrational spectroscopic study of 5-X-uracils and deals with the Raman and IR spectra and vibrational assignments for all the 36 normal modes of vibrations.

2 Experimental

Uracil and 5-aminouracil were purchased from the Aldrich Chemical (USA) and were used as such for spectroscopic studies without any further purification. All the spectra were recorded at room temperature. The Raman spectra (*a* and *b*) of the polycrystalline samples were recorded on a Spex-1877 Raman spectrophotometer in the range 200–4,000 cm^{-1} using the 4,880 Å line from a $\text{C}_w \text{ Ar}^+$ laser as the monochromatic source of excitation, a spectral slit width of 2 cm^{-1} , a constant scan speed of 0.1 cm^{-1}/s and a power less than 100 MW at sample to avoid decomposition of the samples by using a laser-mated beam free from the plasma lines from the incident laser beam. The Raman spectra have appreciable amount of fluorescence background. In such situations, only the strong transitions and not the weak ones may be observed. The data were collected using the DataMate system and were recorded on a chart recorder. The infrared (IR) spectrum (*a*) of uracil powder was recorded in the range 400–4,000 cm^{-1} on a Fourier transform infrared (FTIR) spectrophotometer Model-5300 in Nujol oil. The IR spectrum (*b*) of 5-aminouracil powder was recorded in the range 200–4,000 cm^{-1} on a Perkin-Elmer-883 spectrophotometer using a KBr pellet. The accuracy of the measurement was within $\pm 3 \text{ cm}^{-1}$ and the resolution was better than 2 cm^{-1} for the IR and Raman spectra.

3 Results and Discussion

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 with

Table 1 Fundamental frequencies of uracil and 5-aminouracil

Infrared (FTIR)(cm ⁻¹)		Raman (cm ⁻¹)		Calculated frequencies of parent molecule uracil ^a (cm ⁻¹)	Assignments
(a)	(b)	(a)	(b)		
Uracil	Aminouracil	Uracil	Aminouracil		
Nil	3,380 (s)	Nil	—		<i>a'</i> <i>v</i> _{as} (NH ₂)
Nil	3,290 (m)	Nil	—		<i>a'</i> <i>v</i> _s (NH ₂)
3,180 (m)	3,180 (sh)	—	3,180 (s)		<i>a'</i> <i>v</i> (N ₁ H)
3,160 (m)	3,125 (mw)	—	3,125 (s)		<i>a'</i> <i>v</i> (N ₃ H)
3,095 (m)	Nil	3,100 (w)	Nil	3,067	<i>a'</i> <i>v</i> (C ₅ H)
3,060 (m)	3,070 (sh)	3,065 (s)	3,065 (ms)	3,041	<i>a'</i> <i>v</i> (C ₆ H)
1,735 (vs)	1,755 (s)	1,735 (m)	1,755 (ms)	1,792	<i>a'</i> <i>v</i> (C ₂ =O ₇)
1,705 (vs)	1,715 (sh)	1,680 (vs)	1,715 (w)	1,776	<i>a'</i> <i>v</i> (C ₄ =O ₈)
Nil	1,670 (s)	Nil	1,675 (m)		<i>a'</i> <i>β</i> (NH ₂)
1,650 (vs)	1,650 (s)	1,655 (ms)	1,645 (m)	1,645	<i>a'</i> <i>v</i> (C ₅ =C ₆) ring
1,510 (m)	—	1,510 (ms)	—	1,470	<i>a'</i> <i>β</i> (N ₁ H)
1,450 (s)	1,450 (vs)	1,455 (s)	1,465 (m)	1,470	<i>a'</i> <i>v</i> (ring)
1,410 (vs)	1,420 (vs)	1,410 (vs)	1,420 (s)	1,392	<i>a'</i> <i>β</i> (N ₃ H)
Nil	1,365 (w)	Nil	—		<i>a'</i> <i>v</i> (C ₅ -NH ₂)
1,320 (w)	1,298 (vs)	1,335 (s)	1,310 (s)	1,388	<i>a'</i> <i>v</i> (ring)
1,235 (vs)	1,240 (vs)	1,235 (vs)	—	1,203	<i>a'</i> <i>v</i> (ring) Kekule
—	1,205 (s)	1,180 (m)	—	1,169	<i>a'</i> <i>β</i> (C ₆ H)
Nil	1,100 (ms)	Nil	1,105 (ms)		<i>a'</i> <i>ρ</i> (NH ₂)
1,010 (vs)	1,080 (sh)	1,000 (s)	1,075 (ms)	1,049	<i>a'</i> <i>v</i> (ring)
995 (vs)	1,010 (m)	980 (s)	—	959	<i>a'</i> <i>α</i> (ring)
—	980 (w)	—	975 (ms)	989	<i>a''</i> <i>γ</i> (C ₆ H)
875 (vs)	885 (vs)	880 (s)	885 (m)	940	<i>a''</i> <i>γ</i> (N ₃ H)
820 (s)	843 (m)	835 (ms)	840 (ms)		<i>a''</i> <i>γ</i> (N ₁ H)
785 (sh)	795 (s)	789 (s)	785 (ms)	807	<i>a''</i> <i>γ</i> (C ₂ =O ₇)
775 (s)	768 (vs)	—	—	768	<i>a''</i> <i>γ</i> (C ₄ =O ₈)
740 (sh)	740 (sh)	—	—	738	<i>a'</i> <i>v</i> (ring) breathing
670 (w)	655 (w)	655 (m)	655 (s)		<i>a'</i> <i>α</i> (ring)
630 (w)	600 (sh)	610 (w)	605 (w)	651	<i>a''</i> <i>δ</i> (ring)
570 (m)	555 (vs)	560 (m)	—	542	<i>a'</i> <i>β</i> (C ₂ =O ₇)
540 (m)	530 (sh)	540 (m)	520 (s)	527	<i>a'</i> <i>β</i> (C ₄ =O ₈)
Nil	485 (vs)	Nil	—		<i>a'</i> <i>ω</i> (NH ₂)
Nil	430 (vs)	Nil	430 (ms)		<i>a'</i> <i>τ</i> (NH ₂)
440 (vs)	410 (sh)	450 (m)	—	500	<i>a'</i> <i>α</i> (ring)
—	380 (ssh)	415 (w)	—	382	<i>a''</i> <i>δ</i> (ring)
	280 (s)	260 (s)	283 (ms)	148	<i>a''</i> <i>δ</i> (ring)
Nil	230 (vs)	Nil	—		<i>a'</i> <i>β</i> (C ₅ -NH ₂)
Nil	205 (vs)	Nil	—		<i>a''</i> <i>γ</i> (C ₅ -NH ₂)

vw very weak, *w* weak, *m* medium, *mw* medium weak, *ms* medium strong, *s* strong, *vs* very strong, *sh* shoulder, *ssh* strong shoulder, *v* stretching, *s* symmetric, *as* anti-symmetric, *α* angle bending, *β* in-plane bending, *γ* out-of-plane bending, *τ* torsion/twist, *ρ* rocking, *ω* wagging, *δ* out-of-plane ring deformation or ring torsion

^aThe ab initio calculated frequencies (6-31G basis) for the parent molecule uracil using the GAUSSIAN 90 program [15]

a comparison of theoretically ab initio calculated frequencies using the 6-31G basis set of the GAUSSIAN 90 program. These results are certainly in reasonably good agreement with the experimental IR and Raman spectra for matrix-isolated pyrimidine bases derived from the parent molecule uracil as given in [45]. The parent molecule uracil is known to have a

planar structure both from theoretical [46] and experimental [47] studies in the solid phase. Therefore, to a first approximation, this molecule may be assumed to belong to the C_s point group symmetry, if the NH_2 group is taken to be coplanar with the uracil ring. Under the C_s point group, the distribution of the normal modes between the two species are given by $25a' + 11a''$ of which 30 modes ($21a' + 9a''$) correspond to the uracil moiety and six modes ($4a' + 2a''$) correspond to the NH_2 group as given below:

a' species	a'' species
Symmetric stretching— ν_s (NH_2)	NH_2 wagging— ω (NH_2)
Anti-symmetric stretching— ν_{as} (NH_2)	NH_2 torsion or twist— τ (NH_2)
Symmetric deformation— β (NH_2)	
Anti-symmetric deformations or rocking— ρ (NH_2)	

All of the modes 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. [13, 14, 48] have observed that the skeletal mode of uracil appears to be surprisingly close and, therefore, one might expect a similar pattern for the skeletal modes of the 5-aminouracil. In the assignment of 5-aminouracil modes, assistance has also been taken from studies on uracil [3–44], NH_2 -containing benzene derivatives [49] and substituted uracil [3, 44, 50]. The comparison of theoretically calculated frequencies by the normal coordinate analysis of NH_2 group containing uracil are certainly in reasonably good agreement with the experimental IR and Raman spectra as given in [37]. The assignment of the normal modes of 5-aminouracil is discussed below.

NH_2 Modes The NH_2 group gives rise to six internal modes, namely, symmetric stretching— ν_s (NH_2), anti-symmetric stretching— ν_{as} (NH_2), scissoring or symmetric deformation or simply deformation— β (NH_2), anti-symmetric deformations or rocking— ρ (NH_2), wagging— ω (NH_2) and torsion or twist— τ (NH_2) modes. For aniline and its derivatives, the ν_s , ν_{as} , τ and ω modes are usually localised and are pure group modes whereas the β and ρ modes are mixed with the other ring modes. However, due to the presence of intermolecular hydrogen bonding between the hydrogen atom of the amino group of one molecule and the two oxygen atoms of the two different molecules of the remaining NH_2 group, modes may interact with the other modes in pyrimidine derivatives. In the case of the two NH bonds of the NH_2 group being identical, the ν_s and ν_{as} modes satisfy the relationship $\nu_s = 345.5 + 0.876 \nu_{as}$ as proposed empirically by Bellamy and Williams [51]. For 5-aminouracil, the two NH_2 stretching modes appear at 3,290 and 3,380 cm^{-1} in the IR spectra of each as discussed in [45]. The lower frequency is assigned to the symmetric (ν_s) mode and the higher one to the anti-symmetric (ν_{as}) mode. Using the relation of Bellamy and Williams and taking ν_{as} to be 3,380 cm^{-1} , the ν_s comes out to be 3,306 cm^{-1} which is 16 cm^{-1} more than the observed frequency (3,290 cm^{-1}). In the case of two NH bonds of the NH_2 group being not equivalent, the calculated value of ν_s disagrees with the observed values within ± 2 cm^{-1} . It appears that the two NH bonds of the NH_2 group are not equivalent, due to their involvement and interaction with one hydrogen bond and the other adjacent oxygen atom of the parent molecule.

The scissoring modes (β) of the NH_2 group give rise to its characteristic frequencies in the region 1,600–1,700 cm^{-1} , which contains a broad and strong IR band with peak at 1,670 cm^{-1} as well as a Raman peak of intermediate strength at 1,675 cm^{-1} for 5-aminouracil. The rocking ρ (NH_2) mode usually appears in the region 900–1,150 cm^{-1}

for nucleic acid bases [52, 53]. In the present case, the IR band at $1,100\text{ cm}^{-1}$ is associated with this mode. For 2-thiocytosine, the ω (NH_2) and τ (NH_2) modes have been assigned at 540 and 527 cm^{-1} , respectively, by Beetz and Ascarelli [17]. In fact, the ω (NH_2) and τ (NH_2) modes arise due to the out-of-phase and the in-phase coupling of the two NH out-of-plane bending motions of the NH_2 group. In the assignment of substituted uracil [54], the ω (NH_2) and τ (NH_2) modes have been assigned at 650 and 315 cm^{-1} and also, in the assignment of benzene derivatives [55, 56], assigned near 750 and 400 cm^{-1} , respectively. But 2-thiocytosine [4] has been assigned the ω (NH_2) and τ (NH_2) modes at 804 and 527 cm^{-1} , respectively. Due to its complexity, removal of the ω (NH_2) and τ (NH_2) modes have been performed in parallel studies of substituted uracil [5-X-uracil, X = F, Cl, Br, I, NH_2 and CH_3] with a comparison of ω (NH_2) and τ (NH_2) modes clearly expected at 485 and 430 cm^{-1} compared with the results described in [37].

NH/CH Modes The NH and CH stretching modes usually appear in the region $3,000$ – $3,200\text{ cm}^{-1}$ with the N_1H , N_3H and C_6H stretching modes at higher frequencies, in accordance with the values reported in [3, 6, 26, 57–59]. The Raman band spectrum shows two strong band peaks at $3,180$ and $3,125\text{ cm}^{-1}$ for the N_1H and N_3H stretching modes, respectively, and also one C_6H stretching mode appears with a peak band of intermediate strength at $3,065\text{ cm}^{-1}$, which are given in Table 1, and are in good agreement with [45]. The N_1H , N_3H and C_6H in-plane bending deformations observed at $1,510$, $1,420/1,410$ and $1,205/1,180\text{ cm}^{-1}$, which are in accordance with [3, 4, 58] and also in good agreement with [45], as given in Table 1.

In uracil, out-of-plane NH bending has been assigned in the region 800 – 860 cm^{-1} [20, 39, 50] and I assign the frequencies 840 and 885 cm^{-1} to the γ (N_1H) and γ (N_3H) modes, respectively. One out-of-plane C_6H bending is assigned at 975 cm^{-1} as in [45]; this assignment is similar to that of 2-thiouracil [3].

C–NH₂ Modes According to the crystallography studies of Furberg and Jensen [60], the C– NH_2 bond in 2-thiocytosine ($1.333\text{ \AA}$) is close enough to the C=N bond in the ring ($1.334\text{ \AA}$) and is considerably shorter than the corresponding bond in aniline ($1.42\text{ \AA}$) [61]. The C– NH_2 stretching mode is, therefore, expected to appear at markedly higher frequencies than in aromatic amines. For 5-aminouracil, I assign the frequency $1,365\text{ cm}^{-1}$ to this mode in agreement with the assignment of trifluoromethyl anilines [49] and cytosine [48]. The β (C– NH_2) and γ (C– NH_2) modes for 5-aminouracil are observed with strong band peaks at 230 and 205 cm^{-1} , respectively, which is in close agreement with the assignment of [49] and also nearly associated with the in-plane bending and out-of-plane bending frequencies for 2-thiocytosine [4] at very strong IR band peaks.

C=O Modes The most interesting modes of 5-aminouracil have, out of the six C=O modes, two C=O stretching modes that are easily identified as strong and IR band peaks at $1,715$ and $1,755\text{ cm}^{-1}$, which has also been observed by other authors [3, 6, 15, 17, 22, 23]. Out of the two ν (C=O) modes, the mode due to ν ($\text{C}_4=\text{O}_8$) 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 $\text{C}_4=\text{O}_8$ bond, thereby reducing the magnitude of the ν ($\text{C}_4=\text{O}_8$) mode. The two C=O deformation modes, which have some controversies in the assignment, are expected to be in the region 300 – 900 cm^{-1} . These two β ($\text{C}_2=\text{O}_7$) and β ($\text{C}_4=\text{O}_8$) in-plane bending modes are observed as strong band peaks at 555 and 530 cm^{-1} in IR and for β ($\text{C}_4=\text{O}_8$) at 520 cm^{-1} with strong band peak in Raman.

But, however, some studies of these two C=O in-plane bending modes have led to assignments near 390 and 625 cm^{-1} [17, 20, 48, 62] for uracil and its derivatives. These bends, having similar characteristics, are also observed in both IR and Raman spectra of 5-X-uracils ($X = \text{F}, \text{Cl}, \text{Br}, \text{I}, \text{CH}_3$ and NH_2). The γ (C=O) modes have been proposed near 430 cm^{-1} [17, 20]. In contrast, other studies [26, 32, 45, 58] have proposed the region 680–+ 820 cm^{-1} for these modes, a result supported by the studies from my laboratory. For 5-aminouracil, these bands are observed with very strong peaks at 795 and 768 cm^{-1} and have been correlated to the two γ ($\text{C}_2=\text{O}_7$) and γ ($\text{C}_4=\text{O}_8$) modes. The participation of the O_8 atom in intermolecular hydrogen bonding is expected to make the planar as well as the non-planar $\text{C}_4=\text{O}_8$ motion more difficult compared to the corresponding modes due to the non-bonded one ($\text{C}_2=\text{O}_7$ motion). Hence, the planar and non-planar bending modes due to the $\text{C}_4=\text{O}_8$ bond are expected to have lower magnitude compared to that due to the $\text{C}_2=\text{O}_7$ bond in accordance with [6] and also making a comparison with [45].

Pyrimidine Ring The pyrimidine ring, similar to the phenyl ring, has 12 normal modes of vibration, six of which correspond to ring stretching, three to ring in-plane deformation (α) and three to ring out-of-plane deformation (δ) modes. The stretching modes of the 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 1,650, 1,450, 1,298, 1,240, 1,075 and 740 cm^{-1} . These assignments are in good agreement with those proposed for uracil [32] and its derivatives [3, 4, 6, 45, 50]. The frequency 1,240 cm^{-1} with strong peak could be correlated to the Kekule type vibration mode (ν_{14}) of benzene, whereas the frequency 740 cm^{-1} , showing the similarity to the vibration mode (ν_1) of benzene with a weak IR band peak, is identified as the ring breathing vibration of the pyrimidine ring, similar to that reported in [45].

Similar to benzene and its derivatives [55, 63], 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 modes, 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 deformations are assigned at 982, 559/536 and 516 cm^{-1} by Harsanyi et al. [32], at 802, 548 and 480 cm^{-1} by Colombo and Kirin [58], at 785, 556 and 482 cm^{-1} by Susi and Ard [14], at 995, 732 and 480 cm^{-1} by Szczepaniak et al. [25] and, for 5-trifluoromethyl uracil, at 1,009, 637 and 446 cm^{-1} [6]. In the present case, the frequencies 1,010, 655 and 410 cm^{-1} are assigned to the plane ring deformation in good agreement with the values reported in the literature [6, 10, 25, 32, 45]. The three ring torsional or out-of-plane deformation modes for 1-methyluracil [58], proposed at 525, 445 and 268 cm^{-1} and, for 5-trifluoromethyl uracil, at 602, 418, and 208 cm^{-1} by Shankar et al. [6] are in good agreement with 5-aminouracil of the ring torsional mode frequencies at 600, 380 and 280/283 cm^{-1} in agreement with [45] as given in Table 1.

4 Conclusions

All the 36 normal fundamental modes of 5-aminouracil, which could be assigned in the present case with a comparison of theoretically ab initio calculated frequencies using the 6-31G basis set of the GAUSSIAN 90 program, are certainly in reasonably good agreement with the experimental IR and Raman spectra for matrix-isolated pyrimidine bases derived from the parent molecule uracil as given in [45]. The ring breathing, Kekule and trigonal

angle bending modes are observed to have the same magnitudes as those reported in [45] and for 5-trifluoromethyl uracil. Symmetry and anti-symmetry NH stretching modes of the NH₂ group show the invalidity of the empirical relationship of Bellamy and Williams [51]. These two NH₂ stretching frequencies are distinctly separated from the CH/NH ring stretching frequencies.

Acknowledgements I am grateful to Dr. Asima Pradhan, Department of Physics, I. I. T., Kanpur (India) for recording the Raman spectra in her laboratory.

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