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RAMAN AND INFRARED SPECTRA OF NUCLEIC ACID BASES AND THEIR DERIVATIVES: 5-AMINO-URACIL

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ABSTRACT

Raman and IR spectra of 5-amino-uracil were recorded in the region 200-4000 cm^{-1}. Assuming the molecule under study as a planar one the 36 normal modes are distributed as: 25a' + 11a". Vibrational assignments have been made for all the 36 normal modes with a comparison of theoretically ab initio calculated frequencies using a 6-31G basis set of GAUSSIAN 90 program are certainly in "reasonably good agreement" with the experimental IR and Raman spectra. The two NH bonds of the NH_2 group appear to be equivalent as the NH_2 stretching frequencies satisfy the empirical relation proposed for the equivalent two NH bonds of the NH_2 group. The two NH_2 stretching frequencies are distinctly separated from the CH/NH ring stretching frequencies. A strong and sharp IR band at 3360 cm^{-1} could be identified as the anti-symmetric NH_2 stretching mode whereas the band at 3290 cm^{-1} with smaller intensity could be identified as the symmetric NH_2 stretching mode. All other bands have also been assigned to different fundamentals / overtones / combinations.

Keywords: Infrared spectrum; Raman spectrum; vibrational assignment.

1. INTRODUCTION

Vibrational studies on nucleic acid bases and their derivatives are of considerable importance from biological point of view as these are constituents of genetic materials. Uracil derivatives are used in synthesis of anti-carcinogenic drugs against cancer and anti-HIV viruses. Understanding of the vibrational spectra of 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 [4-27, 45-58]. However, there are still disagreements amongst various workers for the assignments of several modes of uracil. We have done a systematic study of the vibrational spectra of 5-substituted uracils with substituent as NH_2 group for the vibrational spectroscopic investigation. The present article forms Part-I 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 vibration.

2. EXPERIMENTAL

5-amino-uracil was purchased from the Aldrich Chemical Co. (USA) and was used as such for spectroscopic study. All the spectra were recorded at room temperature. Infrared spectrum (Fig.1) of 5-amino-uracil powder was recorded in the range 200-4000 cm^{-1} on a Perkin-Elmer-883 spectrophotometer using KBr optics. IR spectrum (Fig.2) was also recorded at room temperature in the range 600-4000 cm^{-1} on a Perkin-Elmer-1320 spectrophotometer in KBr pellet. The Raman spectrum (Fig.3) of the polycrystalline sample was recorded on a Spex-1877 Raman spectrophotometer in the range 200-4000 cm^{-1} using the 4880 A^0 line from an Ar^+ laser as the source of excitation with the following parameters: 2 cm^{-1} spectral slit width, constant scan speed of 0.1 cm^{-1}/sec. and power less than 100mw at sample to avoid decomposition of the samples. 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 VIBRATIONAL ASSIGNMENTS

The frequencies observed in the IR and Raman spectra along with their relative intensities and proposed vibrational assignments of the fundamental modes are given in Table 1with a comparison of theoretically ab initio calculated frequencies using a 6-31G basis set of GAUSSIAN 90 program are certainly in “reasonably good agreement” with the experimental IR and Raman spectra for matrix isolated pyrimidine bases- parent molecule uracil as given in ref. [46]. Table 2 contains assignment for the lattice modes, overtones and combination bands.

To the best of our information a few structural data are available for 5-amino-uracil in literatures. The parent molecule uracil is known to have a planar structure both from the theoretical [28] and experimental [29] studies in the solid phase. Therefore, to a first approximation the molecule 5-amino-uracil may be assumed to belong to the C_s point group, if the NH_2 group is taken to be coplanar with the uracil ring. Under the C_s point group symmetry the distribution of the normal modes between the two species a’ and a’’ are given by: 25a’+11a”, of which 30 normal modes (21a’+9a”) correspond to the uracil moiety and 6 modes (4a’+2a”) correspond to the NH_2 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. Susi et al. [11, 12, 30] have observed that skeletal modes of uracil appear to be surprisingly close and therefore, one might expect a similar pattern for the skeletal modes of 5-amino-uracil. In the assignment of 5-amino-uracil modes, assistance has also been taken from studies on uracil [1-27], NH_2 containing benzene derivatives [31] and substituted uracil [1, 32]. The assignment of the normal modes of 5-amino-uracil may be discussed under the following sections:

NH_2 group modes, NH/ CH modes, C-NH_2 modes, C=O modes and pyrimidine ring modes.

3.1 *NH_2 group modes*

The NH_2 group gives rise to six internal normal modes, namely, symmetric stretching-$\nu_s(NH_2)$, anti-symmetric stretching-$\nu_{as}(NH_2)$, scissoring or symmetric deformation or simply deformation - $\beta(NH_2)$, anti-symmetric deformation or rocking- $\rho(NH_2)$, wagging- $\omega(NH_2)$ and torsion or twist- $\tau(NH_2)$ modes. For aniline and its derivatives the $\nu_{s,}$ $\nu_{as,}$ ω and τ modes of the NH_2 group are usually localized and are pure group modes where as the β and ρ modes mix up with the other ring modes. However, due to the presence of intermolecular hydrogen bonding between hydrogen atom of the amino group of one molecule and the two oxygen atoms of the two different molecules the remaining NH_2 group modes may interact with the other modes in pyrimidine derivatives. In the case of two NH bonds of the NH_2 group being identical the ν_s and ν_{as} modes satisfy the relationship $\nu_s = 345.5+0.876\ \nu_{as}$ empirically proposed by Bellamy and Williams [33]. For 5-amino-uracil the two NH_2 stretching modes appear at 3290 and 3360 cm^{-1} in the infrared spectra. 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 at 3360 cm^{-1}, the ν_s comes out to be 3289 cm^{-1} which is only 1cm^{-1} lower than observed frequency (3290 cm^{-1}). In the case of two NH bonds of the NH_2 group being equivalent the calculated value of ν_s agrees with the observed values within ± 2cm^{-1}. It appears that the two NH bonds of NH_2 group are equivalent. The scissoring modes (β) of the NH_2 group gives rise to its characteristic frequencies in the region 1600-1700 cm^{-1} which contains a broad and strong IR band with peak at 1670 cm^{-1} for 5-amino-urail. The rocking ρ (NH_2) mode usually appears in the region 900-1150 cm^{-1} for nucleic acid bases [34, 35]. In present case the IR band at 1100 cm^{-1} is associated with this mode. For 2-thiocytocine the ω (NH_2) and τ (NH_2) modes have been assigned at 540 and 527cm^{-1} by Beetz and Ascarelli [36]. In fact 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 [37] of the ω (NH_2) and τ (NH_2) modes have been assigned at 650 and 315 cm^{-1} and also in the assignment of [38, 39] assigned at near 750 and 400 cm^{-1}. But the assignment [2] of 2-thiocytosine has been assigned the ω (NH_2) and τ (NH_2) modes at 804 and 527 cm^{-1}. Due to remove the complexity in ω (NH_2) and τ (NH_2) modes have 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 ω (NH_2) and τ (NH_2) modes are clearly expected at 485 and 430 cm^{-1}.

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, 40-42, 51-58]. The Raman spectrum shows two strong bands at 3180 and 3125 cm^{-1} which could be assigned to the N_1H and N_3H stretching modes respectively. A medium strong band appears at 3065 cm^{-1} which we assign as the C_6H stretching mode. The N_1H, N_3H and C_6H in-plane bending deformations are observed at 1580, 1420 and 1205 cm^{-1} respectively in accordance with [1, 2, 41].

In uracil, the out-of-plane NH bending have been assigned in the region 800-860 cm^{-1} [18, 32, 41] and we assign the frequencies 840 and 885 cm^{-1} to the $\gamma(N_1H)$ and $\gamma(N_3H)$ modes respectively. The C_6H out-of-plane bending is assigned at 975 cm^{-1} in agreement with the earlier assignment for this mode for 2-thiouracil [1].

3.3 *C-NH_2 modes*

According to the crystallography studies Furberg and Jensen [43] the C-NH_2 bond in 2-thiocytosine ($1.333A^0$) is close enough to the C=N bond in the ring ($1.334A^0$) and is considerably shorter than the corresponding bond in aniline (1.42A^0) [44]. The C-NH_2 stretching mode is, therefore, expected to appear at markedly higher frequency than in aromatic amines. For 5-amino-uracil, the frequency 1365 cm^{-1} is assigned to this mode in agreement with the assignment proposed earlier [38]. The β(C-NH_2) and γ(C-NH_2)modes for the 5-amonouracil are observed as strong bands at 230 and 205 cm^{-1} whose assignments are in close agreement with published literature [31].

3.4 *C=O modes*

The most interesting modes of 5-amino-uracil are the two C=O stretching, the two C=O in-plane bending and the two C=O out-of-plane bending modes. The C=O stretching modes are easily identified as strong IR bands at 1715 and 1755 cm^{-1} in agreement with the earlier assignments made for these modes in related molecules[1, 4, 15, 20, 21, 51-57]. 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 which weaken the C_4=O_8 bond thereby reduces the magnitude of the ν(C_4=O_8) mode. There are some controversies in the assignments of the two C=O deformation modes which are expected to appear in the region 300-900 cm $^{-1}$. These two modes β (C_2=O_7) and β (C_4=O_8) are observed in IR as strong bands at 555& 530 cm^{-1}. However, in Raman spectrum the band due to β (C_4=O_8) appears at 520 cm^{-1} with strong intensity. However, some workers have been assigned these two C=O in-plane bending modes for uracil and its derivatives near at ~390 and ~625 cm^{-1} [15, 18, 30]. These bands having similar characteristic are also observed in both the IR and Raman spectra of 5-X-uracils (X=F, Cl, Br, I, and CH_3). The γ (C=O) modes have been proposed near 430 cm^{-1} by some workers [15, 18] whereas some other workers [24, 41, 45] have proposed these modes in the region 680-820 cm^{-1}. We agree with the assignments of the latter group of workers. For the 5-amino-uracil these bands are observed with very strong peaks at 795 and 768cm^{-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 make the planar as well as the non-planar C_4=O_8 motion 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 1650, 1450, 1298, 1240, 1075 and 740 cm^{-1}. Assignments for these modes are is good agreement with those proposed for uracil [45] and its derivatives [1, 2, 4, 32, 51-58]. The frequency 1240 cm^{-1} with strong peak could be correlated to the Kekule type vibration mode (ν_{14}) of benzene whereas the frequency 740 cm^{-1}, having character similar to that of ν_1 of benzene 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 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 has Harsanyi et al. [45], at 802, 548 and 480 cm^{-1} by Colombo and Kirin [41], at 785, 556 and 482 cm^{-1} by Susi and Ard [12], at 995, 732 and 480 cm^{-1} by Szczesniak et al. [23] and at 1009, 637 and 446 cm^{-1} by Shankar et al. [4]. In the present case the frequencies 1010, 655 and 410 cm^{-1} are assigned to the in-plane ring deformation mode in agreement with the earlier workers [4, 8, 23, 45]. For 1-methyluracil [41] the three ring torsional or out-of-plane deformation modes have been proposed at 525, 445, and 268 cm^{-1} and for 5-trifluoromethyluracil [4] at 602, 418, and 208 cm^{-1} . In the present case the ring torsional modes are assigned at the frequencies 600, 380 and 280/283 cm^{-1}.

4. CONCLUSIONS

Here, all the 36 normal modes of 5-amino-uracil could be assigned in the present case with a comparison of theoretically ab initio calculated frequencies of parent molecule uracil using a 6-31G basis set of GAUSSIAN 90 program are certainly in “reasonably good agreement” with the experimental IR and Raman spectra for matrix isolated pyrimidine bases as given in ref. [46]. The ring breathing, Kekule and trigonal angle bending modes are observed to have nearly same magnitudes as for 5-trifluoromethyluracil [4], 5-methyl-uracil (thymine) [51] 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 as well as some where it is found that a need of modification in their frequencies magnitudes of the works [47-58]. Similarly, all the C=O modes are observed at nearly same frequencies as for 5-trifluoromethyl uracil. Symmetric and anti-symmetric NH_2 stretching modes of the NH_2 group show the validity of the empirical relationship of Bellamy and Williams [33].

REFERENCES

[1] R. A. Yadav, P.N.S. Yadav and J.S.Yadav, *Proc. Ind. Acad. Sci. (Chem Sci.)* **100**, 69 (1988).

[2] R. A. Yadav, P.N.S. Yadav and J.S. Yadav, *Spectrochim. Acta.* **44 A**, 1201 (1988).

[3] K. Singh, R. A. Yadav and J.S. Yadav, *Spectrochim. Acta* **47A,** 816 (1991).

[4] R Shankar, R. A. Yadav and I.S. Singh, *Spectrochim. Acta* **50A**, 1251 (1994).

[5] E.R. Blout and M. Fields, *J. Am. Chem. Soc.* **72**, 479 (1950).

[6] L .N. Short and H.W. Thompson, *J. Chem. Soc.*168 (1952).

[7] J.R. Lacher, J.L. Bitner, D.J. Emery, M.E. Sefel and J.D. Park, *J. Chem. Phys*. **59,** 615 (1955).

[8] C.L. Angell, *J. Chem. Soc.* 504 (1961).

[9] T. Shimanouchi and I. Harada, *J. Chem. Phys*. **41,** 2651 (1964).

[10] R.C. Lord and J.G. Thomas, Jr., *Spectrochim. Acta* **23A,** 2551 (1967).

[11] H. Susi and J.S. Ard, *Spectrochim. Acta* **27A,** 1549 (1971).

[12] H. Susi and J.S. Ard, *Spectrochim. Acta* **30A**, 1843 (1974).

[13] M.J. Nowak, K. Szczepaniak, A. Barski and D. Shugar, Z. *Naturforsch.* **C33**, 876 (1978).

[14] G. Bardi, L. Bencivenni, D. Ferro, B. Martini, S. Nunziante-Cesaro and R. Teghil, *Thermochim. Acta* **40,** 275 (1980).

[15] C.P. Beetz. Jr. and G. Ascarelli, *Spectrochim. Acta* **36A,** 299 (1980).

[16] W.D. Bowman and T.G. Spiro, *J. Chem. Phys.* **73**, 5482 (1980).

[17] M. Shibata, T.J. Zielinski and R. Rein, *Int. J. Quantum Chem.* **18,** 323 (1980).

[18] J. Bandekar and G. Zundel, *Spectrochim. Acta* **38A**, 815 (1982).

[19] A.W. Espinoza-Muller and A.N. Bravo, *J. Mol. Struct.* **90,** 187 (1982).

[20] J. Bandekar and G. Zundel, *Spectrochim Acta* **39A**, 337 (1983).

[21] J. Bandekar and G. Zundel, *Spectrochim, Acta* **39A**, 343 (1983).

[22] E.D. Radchenko, A.M. Plokhotnichenko, g.G. Sheina and Yu. P. Blagoi, *Biofizika* **28,** 923 (1983).

[23] M. Szczesniak, M. J. Nowak, H. Rostkowska, K. Szczepaniak, W. B. Person and D. Shugar, *J. Am. Chem. Soc.* **105**, 5969 (1983).

[24] A.J. Barnes, M.A. Stuckey and L. Le Gall, *Spectrochim. Acta* **40A,** 419 (1984)

[25] S. Chin, V. Scott, K. Szczepaniak and W.B. Person, *J. Am. Chem. Soc.* **106,** 3415 (1984).

[26] M. Maltese, S. Passerini, S. Nunziante-Cesaro, S. Dobos and L. Harsanyi, *J. Mol. Struct.* **116**, 49 (1984).

[27] K. Szczepaniak, M. Szczesniak, M. J. Nowak, I. Scott and W. B. Person, *Int. J. quantum Chem. Symp.* **18**, 547 (1984).

[28] A. Buda and A. Syguta, *J. Mol. Struct.* **92,** 255 (1983).

[29] R.F. Stewart and L.H. Jensen, *Acta Cryst.* **23 ,** 1102 (1967).

[30] H. Susi T.S. Ard and J. M. Purcell, *Spectrochim. Acta* **29A**, 725 (1973).

[31] D. N. Singh, R. Shankar, R. A. Yadav and I. S. singh, *J. of Raman Spectrosc.* **27,** 177 (1996).

[32] S. Aruna and G. Shanmugam, *Spectrochim, Acta* **41A,** 531 (1985).

[33] L.J. Bellamy and R.L. Williams, *Spectrochim. Acta* **9A,** 341 (1957).

[34] J. M. Delabar and M. Majoube, *Spectrochim. Acta* **34 A,** 129 (1978).

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

[36] C. P. Beetz, Jr. and G. Asarelli , *Spectrochim. Acta* **36A,** 299 (1980).

[37] R. Shankar, R. A. Yadav, I. S. Singh and O. N. Singh, Pramana **24**, 749 (1985).

[38] R.A. Yadav, Ph.D. Thesis, Banaras Hindu University, India (1983).

[39] R. Shanker, R.A. Yadav, I.S. Singh and O.N. Singh, *J. Raman Spectrosc.* **23,** 141 (1992).

[40] R.A. Yadav and I.S. Singh, *Proc. Ind. Acad. Sci. (Chem.. Sci.)* **95,** 471 (1985).

[41] L. Colombo and D. Kirin, *Spectrochim, Acta* **42A,** 557 (1986).

[42] D.N. Sathyanarayana and S. V. Kasmir Raja, *Spectrochim. Acta* **41A,** 809 (1985).

[43] S. Furberg and L. H. Jensen, *Acta Crystallogr.* **B 26**, 1260 (1970).

[44] H. J.M. Bowen, J. Donohue, D.J. Jenkin, O. Kennard, P.T. Wheatley and D.H. Whiffen , *Chem. Soc*. (Londan) Spect. Publ. 11, 377 (1958).

[45] L. Harsanyi, P. Csaszar, A. Csaszar and J.E. Boggs, *Int. J. Quantum Chem*., **29**, 799 (1986).

[46] J.R. Durig, in *Vibrational Spectra and Structure* (Edited by J.R. Durig), Vol. 20, pp. 285-325. Elsevier science Publ.ishers, The Netherlands (1993).

[47] M. Alcolea Palafox¸ V. K. Rastogi , *Spectrochim. Acta* **58A,** 411 (2002).

[48] Billinghurst, B. E., Yeung, R., and Loppnow, G. R. **,** *J. Phys. Chem.* **A 110,** 6185 (2006).

[49] Soujanya Yarasi, Brant E. Billinghurst, Glen R. Loppnow **,** *J. Raman Spectrosco* .**38**, 1117 (2007).

[50] Yarasi, S., Brost, P., and Loppnow, G. R.**,** *J. Phys. Chem***. A 111**, 5130 (2007).

[51] J. S. Singh, *J. Mol. Struct*. **876,** 127 (2008).

[52] J. S. Singh**,** *Spectrosc. Lett.* **41,** 122 (2008).

[53] J. S. Singh**,** *Pramana – J. Phys.* **70** (3), 479 (2008).

[54] J. S. Singh**,** *J. Bio. Phys.* **34,** 569 (2008).

[55] J. S. Singh**,** *Spectrochim. Acta* A (G.B.), **87,** 106 (2012).

[56] J. S. Singh, *Spectrochim. Acta* A (G.B.), **117,** 502 (2013).

[57] J. S. Singh, *Spectrochim. Acta* A (G.B.), **130,** 313 (2014).

[58] J. S. Singh, *Spectrochim. Acta* A (G.B.), **137**, 625 (2015).

Table1.Fundamental frequencies* of 5-amino-uracil

Infrared cm^{-1}		Raman cm^{-1} (Fig. 3)	Calculated frequencies of parent molecule uracil[a] (cm^{-1})	Assignments[$]	
PE-1320 (Fig. 2)	PE-883 (Fig. 1)				
3360(vs)	3360(s)	----		a’	$\nu_{as}(NH_2)$
3290(ssh)	3290(m)	-----		a’	$\nu_s(NH_2)$
3180(sh)	3180(sh)	3180(s)		a’	$\nu(N_1H)$
-----	3125(mw)	3125(s)		a’	$\nu(N_3H)$
3075(m)	3070(sh)	3065(ms)	3041	a’	$\nu(C_6H)$
1755(ssh)	1755(s)	1755 (ms)	1792	a’	$\nu(C_2=O_7)$
1715(ssh)	1715(sh)	1715(w)	1776	a’	$\nu(C_4=O_8)$
1670(ssh)	1670(s)	1675(m)		a’	$\beta(NH_2)$
1650(ssh)	1650(s)	1645(m)	1645	a’	$\nu(C_5=C_6)$ ring
1580(m)	1580(s)	1580(s)	1470	a’	$\beta(N_1H)$
1445(vs)	1450(vs)	1465(m)	1470 (mixing)	a’	ν (ring)
1420(vs)	1420(vs)	1420(s)	1392	a’	$\beta(N_3H)$
-----	1365(w)	-----		a’	$\nu(C_5-NH_2)$
-----	1298(vs)	1310(s)	1388	a’	ν (ring)
1240(vs)	1240(vs)	----	1203	a’	ν (ring) Kekule
1205(vs)	1205(s)	----	1169	a’	$\beta(C_6H)$
1100(vs)	1100(ms)	1105(ms)		a’	$\rho(NH_2)$
-----	1080(sh)	1075(ms)	1049	a’	ν (ring)
1010(vs)	1010(m)	----	959	a’	α (ring)
980(sh)	980(w)	975(ms)	989	a”	$\gamma(C_6H)$
880(s)	885(vs)	885(m)	940	a”	$\gamma(N_3H)$
845(sh)	843(m)	840(ms)		a”	$\gamma(N_1H)$
790(s)	795(s)	785(ms)	807	a”	$\gamma(C_2=O_7)$
760(s)	768(vs)	----	768	a”	$\gamma(C_4=O_8)$
740(sh)	740(sh)	----	738	a’	ν (ring)-breathing
655(w)	655(w)	655(s)		a’	α (ring)
600(w)	600(sh)	605(w)	651(mixing)	a”	δ (ring)
	555(vs)	-----	542	a’	$\beta(C_2=O_7)$
	530 (sh)	520(s)	527	a’	$\beta(C_4=O_8)$
	485(vs)	------		a”	$\omega(NH_2)$
	430(vs)	430(ms)		a”	$\tau(NH_2)$
	410(sh)	----	500	a’	α (ring)
	380(ssh)	-----	382	a”	δ (ring)
	280(s)	283(ms)	148	a”	δ (ring)
	230(vs)	----		a’	$\beta(C_5-NH_2)$
	205(vs)	----		a”	$\gamma(C_5-NH_2)$

[*] vw = very weak, w = weak, m = medium, mw = medium weak, ms =medium-strong, s =strong, vs = very strong, sh = shoulder, ssh =strong shoulder. [$] ν: 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.

[a] The ab initio calculated frequencies (6-31G basis) for the parent molecule uracil using GASSIAN 90 program in ref.[46]

Table2. Lattice modes, overtones and combination frequencies of 5-amino-uracil

IR cm^{-1}	IR cm^{-1}	Raman cm^{-1} (Fig. 3)	Assignments
PE-883 (Fig. 1)	PE-1320 (Fig. 2)		
	3000(sh)		1420+1580
		2985(mw)	1310+1675
2880(ms)		2880(w)	1420+1460
		2840(mw)	2 x 1420
2820(ms)	2820(s)		1240+1580
2450(w)	2445(s)		1450+1010
2020(m)	2020(m)		2 x 1010
1980(w)			1420+555
1950(w)	1950(s)		1420+530
1500(m)	1500(sh)	1500(m)	1080+410, 2 x ring stretching
380(w)			Intermolecular / lattice
300(s)			Intermolecular / lattice

*Abbreviations are similar to those defined in Table 1.

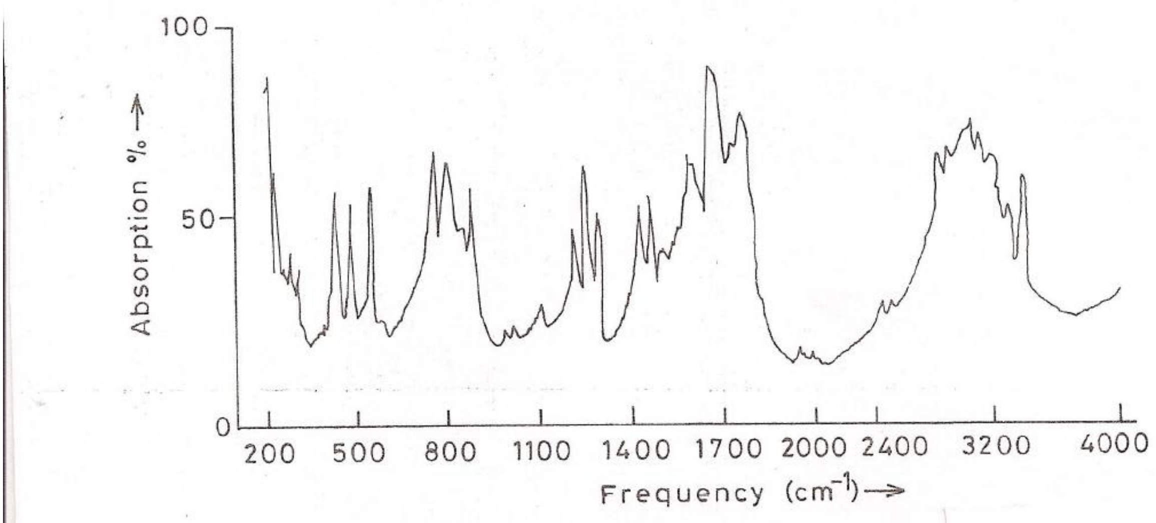

FIG. 1 INFRARED SPECTRUM OF 5-AMINO URACIL

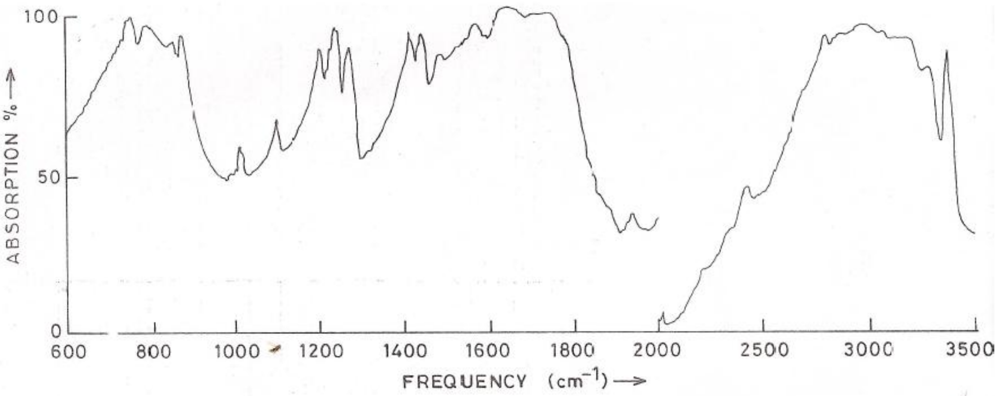

FIG. 2 INFRARED SPECTRUM OF 5-AMINO URACIL

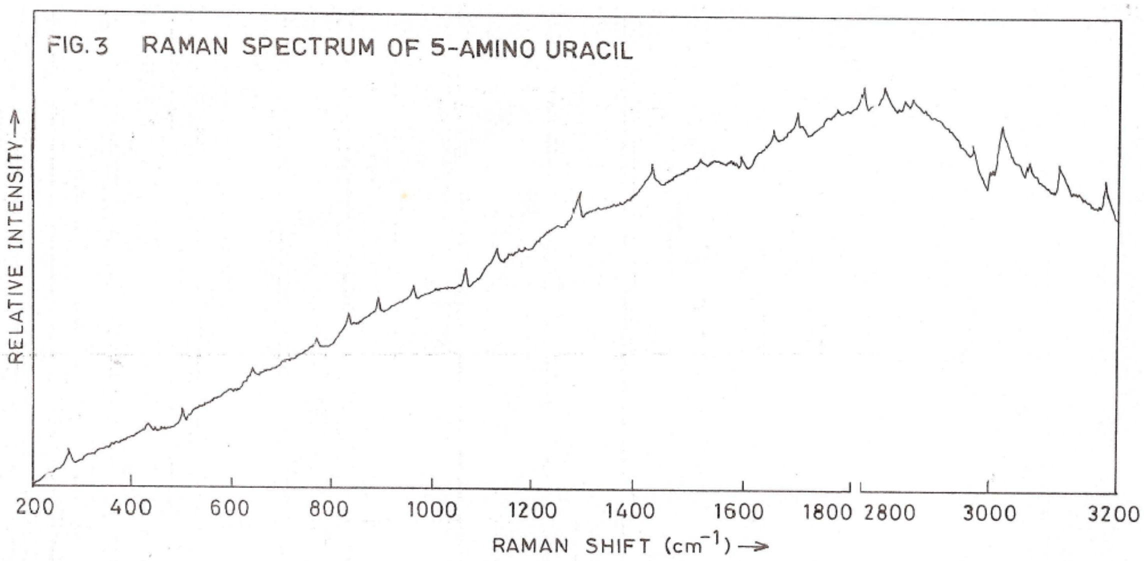

FIG. 3 RAMAN SPECTRUM OF 5-AMINO URACIL