

Vibrational spectra of 4,6-Diamino-2-Hydroxy Pyrimidine

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ABSTRACT

The study of N-Heterocyclic molecules is of great importance and has become more relevant due to their biological and pharmaceutical utility workers have carried out spectral investigations of these molecules. The vibrational spectra of these compounds provide evidences about outstanding structural problems. One of them is tautomerism which arises due to the involvement of functional groups and may affect their function in the metabolism. Bio-physical research requires a good understanding of the vibrational spectra of nucleic acid base. The special studies of nucleic acid bases and their derivatives containing pyrimidine moieties have been carried out both experimentally and theoretically. The vibrational spectra of various substituted pyrimidines was studied by many workers. Some workers had predicted theoretically the absorption spectra of uracil and cytosine nucleosides. In view of these, the Laser Raman and I.R. spectrum of 4,6-Diamino-2-Hydroxy pyrimidine have been recorded in 100-400 cm^{-1} 200-400⁻¹ (By KBr pallet technique) region.

INTRODUCTION:

The study of pyrimidines and substituted pyrimidines in N-Heterocyclic molecules is of great importance and has become more relevant due to their biological and pharmaceutical utility workers (Anderson et al 2014, Eihatty et al 1990, Goel et al 1986, Guarner et al 2006, Gupta et al 1990, Hong et al 2004, Kim et al 2008 and Szymansky et al 1964) have carried out spectral investigations of such molecules. The vibrational spectra of these compounds provide evidences about outstanding structural problems. One of them is tautomerism which arises due to the involvement of functional groups like OH-NH, -SH and may affect their function in the metabolism. Bio-physical research requires a good understanding of the vibrational spectra of nucleic acid base (Anderson et al 2014, Bernhard 1995, Jacque et al 1970 and Szczesniak et al 1985). In substituted pyrimidines the position of substituents, their tautomeric behavior and hydrogen bonding ability of C-

O bond is considerable biological evidence. The special studies of nucleic acid bases and their derivatives containing pyrimidine moieties have been carried out both experimentally and theoretically. The vibrational spectra of various substituted pyrimidines were studied by some workers (Chand^a et al 2021, Jacque et al 1970 and Leila et al 2016). Some workers (Anderson et al 2014, Deep et al 2013, Mariani et al 2012 and Szesesniak et al 1985) also studied in a comprehensive way the vibrational spectra of derivatives of pyrimidine with group analysis and tautomeric behavior. So, considering the above facts, the work was undertaken with the aim of studying the infrared and laser Raman spectra of 4,6-Diamino-2-hydroxy Pyrimidine.

EXPERIMENTAL DETAILS: The spec-pure grade sample of 4,6-diamino-2-hydroxy pyrimidine (hereafter referred to as 4,6,2-DAHP) was obtained readymade and used as such after confirming the purity of the said molecule by elemental analysis as well as melting point determination. The infrared spectra of 4,6,2-DAHP has been recorded in the region 200-400 cm^{-1} using KBr Pallet technique. The laser Raman spectrum was recorded, using 4880 Å line of Ar^+ in the region of 400-100 cm^{-1} in Carry-Model-82 grating spectrophotometer by using 4 watt Ar^+ laser light.

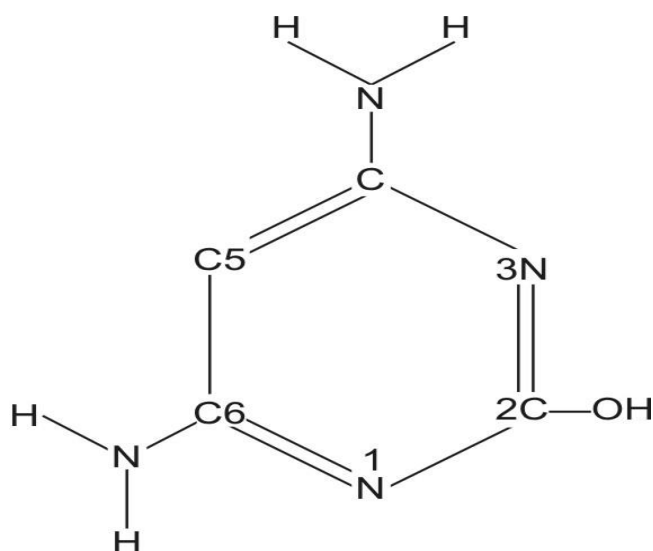


Figure 1: The molecular structure of 4,6-Diamino-2-Hydroxy pyrimidine

RESULT AND DISCUSSION:

The structure of various pyrimidines (Compounds) has been determined and in all cases the molecules were found to be planar. Assuming amino and hydroxyl groups as a single mass points, the molecule 4,6,2-DAHP belongs to C_{2v} , non planar. The study is based on

the magnitudes and relative intensities of the observed bands and the assignments in related molecules.

The molecular Structure of 4,6-Diamino-2-Hydroxy pyrimidine is shown in Figure 1. The infrared and laser Raman spectra of 4,6,2-DAHP are given in the Figure 2 and 3 respectively. The observed vibrational frequencies of infrared and laser Raman Spectra are given in the Table 1 along with intensities. The correlation of amino-group is given in Table 2. The detailed discussion of the spectra of the said molecule is given as under.

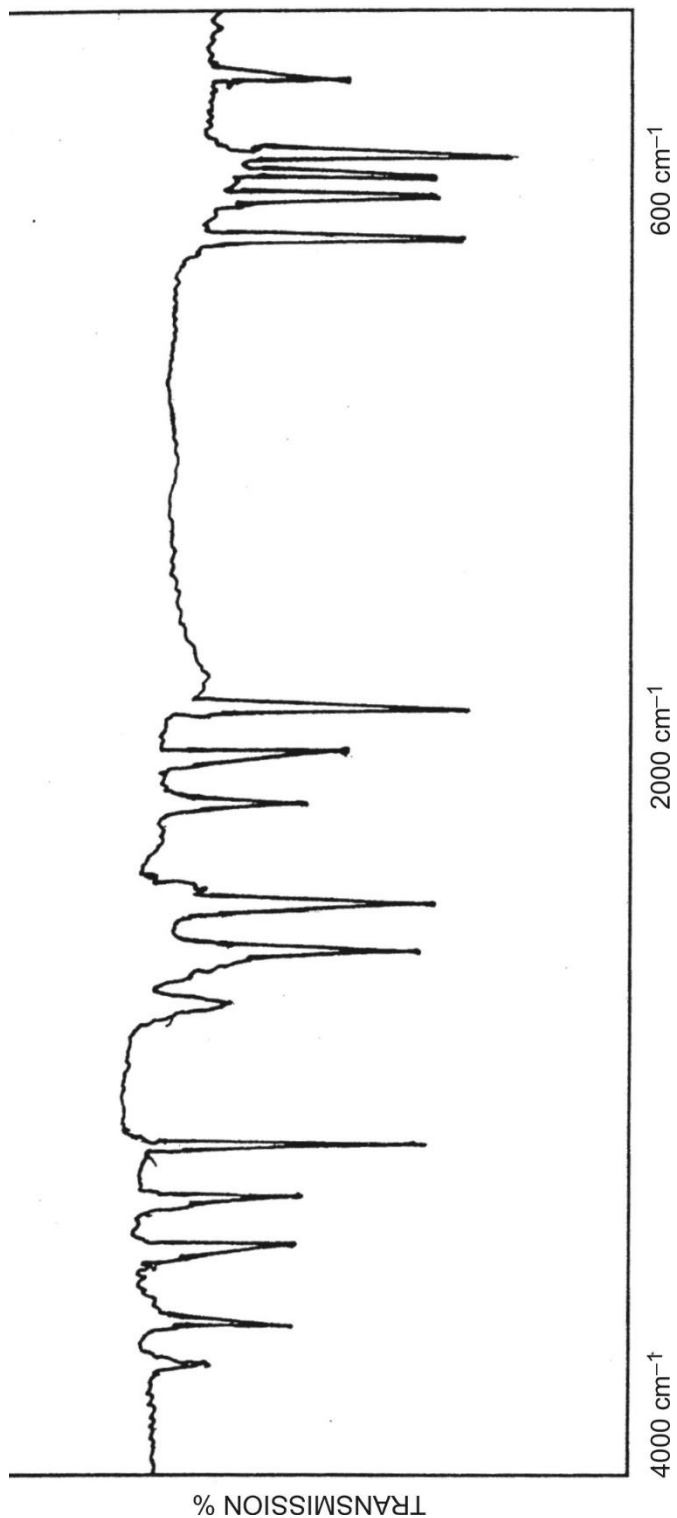


Figure 2: Infrared Spectrum of 4, 6, 6, 6 DAHP

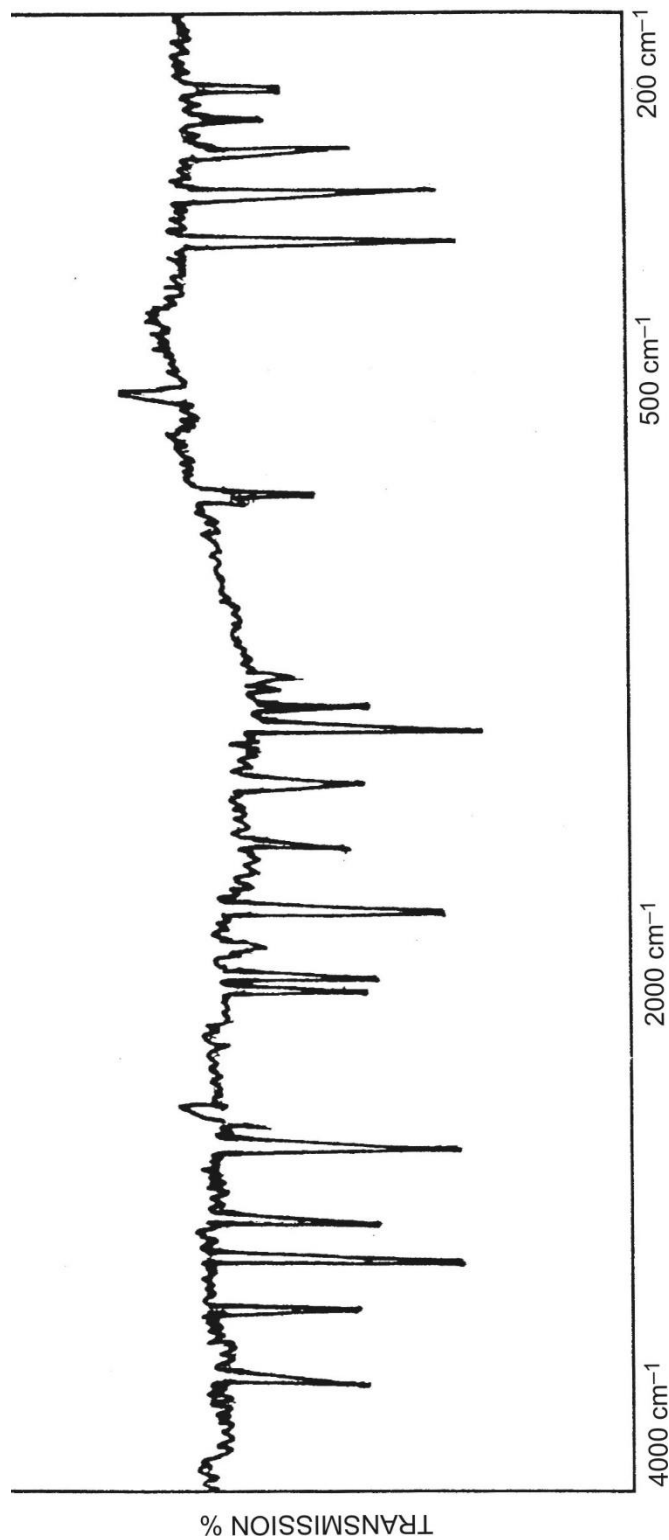


Figure 3: Laser Raman Spectrum of 4, 6, 2 DAHP

TABLE 1

**Assignments of Fundamental Frequency of
4,6,2-DAHP (All Values in cm^{-1})**

Assignments	Pyrimidine	Infrared Spectra (Frequency & Intensity)	Raman Spectra Frequency & Intensity)
Ring breathing, $\nu(\text{C—C})$	990	760 vvs	790 vs
$\nu(\text{C—H})$	3055	1338 vw	—
$\beta(\text{C—H})$	1230	1135 vw	1115 w
$\beta(\text{OH})$	—	1145 s	1160 s
$\gamma(\text{C—C})$	710	708 w	698 w
$\gamma(\text{C—OH})$	—	330 ms	326 ms
$\beta(\text{C—C})$	680	588 w	570 w
$\beta(\text{C—C})$	—	610 w	625 w
NH_2 wagging	—	645 w	640 w
NH_2 wagging	—	655 ms	685 ms
$\nu(\text{C—NH}_2)$	3085	1350 ms	1385 w
$\nu(\text{CC})(\text{CC})$	1564	1570 w	1550 w
$\nu(\text{CC})(\text{CC})$	1568	1610 vvs	1600 vvs
NH_2 Scissoring	—	1650 ms	1655 ms
NH_2 Scissoring	—	1675 ms	1660 ms
$\nu(6\text{C}=\text{O})$	—	1685 s	1690 w
$\beta(\text{C—OH})$	—	570 vs	566 w
$\gamma(\text{C—H}_2)$	—	—	250 w
NH_2 Torsion	—	—	195 w
$\gamma(\text{C—H})$	815	800 w	850 w
$\beta(\text{C—H})$	1070	940 vw	985 w
NH_2 Twisting	—	1055 ms	1035 s
Assignments	Pyrimidine	Infrared Spectra (Frequency & Intensity)	Raman Spectra (Frequency & Intensity)

		Intensity)	
NH ₂ Twisting	—	1105 vvw	1100 ms
$\nu(\text{C—OH})$	—	1235 vvs	1260 vvs
$\nu(\text{C—C})$	—	1320 vvw	1295 w
$\beta(\text{C—NH}_2)$	1159	— 385 vw	360 w
$\gamma(\text{OH})$	—	— 385 vw	380 w
$\gamma(\text{C=H})$	—	395 vw	400 ms
$\nu(\text{C—C})$	310	400 s	445 ms
$\gamma(\text{C=O})$	—	550 vw	560 w
$\nu(\text{C—C})$	340	709 w	345 w
$\beta(\text{C—NH}_2)$	1075	345 vvw	—
$\gamma(\text{C—NH}_2)$	—	—	235 w
$\nu(\text{OH—O})$	—	—	155 w
$\nu(\text{C—C})(\text{C—N})$	1400	1405 ms	1455 ms
$\nu(\text{C—C})(\text{C—N})$	1466	1520 vvs	1495 vs
$\nu(\text{C—H})$	3070	3060 vvs	3045 vs
$\nu(\text{NH})$ symn.	—	3245 vs	3260 vs
$\nu(\text{NH—N})$	—	3295 vvw	—
$\nu(\text{NH})$ symm.	—	3330 vs	3305 s
$\nu(\text{NH})$ asymn.	—	3405 vs	3434 s
$\nu(\text{NH})$ asymn.	—	3582 vw	3556 w
$\nu(\text{OH})$	—	3662 vw	3624 w

Where ν = Stretching β = in-plane-bending γ = out-of-plane-bending

ms = medium strong s = strong vs = very strong

vvs = very very strong w = weak vw = very weak

vvw = very very weak

TABLE 2
Correlation of Amino Group Vibrations
4,6,2-DAHP with Similar Molecules
(All Values in cm⁻¹)

Assignments	2,4,6-TAP (a)	Aniline (b)	2,4,6-ADMP (c)	4,2,6-ADMP (d)	4,6,2-DAHP (t)	
					IR	Raman
$\nu(\text{NH})$ asymn	—	—	—	—	3570	3550
$\nu(\text{NH})$ asymn	3430	3435	3420	—	3410	3445
$\nu(\text{NH})$ asymn	3319	3360	3320	3340	3320	3295
$\nu(\text{NH})$ asymn	—	—	—	—	3250	3260
NH ₂ scissoring	1660	—	—	1670	1680	1672
NH ₂ scissoring	—	1620	1642	—	1650	1645
NH ₂ twisting	1094	—	—	—	1105	1100
NH ₂ twisting	—	1054	1048	1040	1060	1040
NH ₂ wagging	648	—	—	—	655	685
NH ₂ wagging	—	570	560	555	645	640

Where ν = stretching, asym = asymmetric,

Symm = symmetric, t = Present molecule

VIBRATIONAL SPECTRUM: Pyrimidine has three C-H stretching modes one belonging to the a_1 species and one belonging to the b_2 species. Bellamy (1975) and Rao (1963) assigned the C-H stretching modes in pyrimidine in the region 3000 – 3100 cm⁻¹ on substitution at 4 and 6 positions, the mode ν^{13} and ν_{7b} drop in accordance with the assignments given by some workers (Krishnakumar et al 2008, Kumar^c et al 2021 and Nejad et al 1975).

For pyrimidines 4,6- $d_2\nu_{13}$ and ν_{7b} modes drop where substitutions are made at 4 and 6 positions. Thus, the bands observed at 3060 cm⁻¹ and 3045 cm⁻¹ in I.R. and Laser Raman spectra have been assigned to C-H stretching mode ν_{20} a. Sanyal et al (1979) have assigned this mode at 3109 cm⁻¹ in KBr and at 3109 cm⁻¹ in Nujomull in case of 2,4,6-triamino pyrimidine while others (Mohan et al 1994, Silverstain et al 1991 and Venkatraman et al 2019) assigned this mode at 3080 cm⁻¹ in case of substituted heterocyclic compounds.

The weak band observed at 1135 and 1115 cm^{-1} in infrared and laser Raman spectra have been assigned β_3 vibration corresponding to C-H in plane-bending mode. Goel et al (1986) assigned this mode very well at 1204 cm^{-1} in 4,6-dihydroxy pyrimidine. The C-H out of plane bending mode γ_{11} , have been assigned at 800 and 850 cm^{-1} infrared and laser Raman spectra. These assignments also find support from the literature value (Arieh 2008, Anderson et al 2014, Bersani et al 2010, Deep et al 2013, Eihaty et al 1990, Goel et al 1986, Guarner et al 2006, Gupta et al 1990, Hong et al 2004, Ingold 1953 and Szesesniak et al 1985).

The pairs of absorption bands at 1400(ν_{19a}), 1466(ν_{19b}) cm^{-1} and at 1564(ν_{8a}) and 1568(ν_{8b}) have been observed in the spectra of pyrimidine (Kumar^c et al 2021, Najad et al 1975 and Yadav^{a-c} et al 1997). These are analogous to the pairs of bands originating from e_{14} (1485) and 2_{eg} (1595) modes of benzene observed in substituted benzenes (Anderson et al 2014, Deep et al 2013, Eihaty et al 1990, Guarner et al 2006, Gupta et al 1990, Hong et al 2020, Ingold 1953, Jacque et al 1970 and Szczesniak et al 1985). The ν_{19a} band is observed at 1382 cm^{-1} in 2-chloro pyrimidine (Bellamy 1975 and Sharma et al 1980) and at 1391 cm^{-1} in 5 methyl pyrimidine (Kumar 2000). Some workers (Anderson et al 2014, Deep et al 2013, Eihaty et al 1990, Frankiss et al 1976, Goel et al 1986, Gupta et al 1990, Jacque et al 1970 and Schrader et al 1995) assigned the modes at 1420, 1490, 1590 and 1620 cm^{-1} to C-C stretching vibrations so bands ν_{19a} , ν_{19b} and ν_{8a} and ν_{8a} have been assigned at 1405, 1520, 1570 and 1610 cm^{-1} in the infrared spectra and at 1455, 1495, 1550, 1600 cm^{-1} in Raman spectra of the mentioned molecule respectively are analogous to the spectra of substituted benzenes. These bands are due to the double bond $\text{C}=\text{C}$ and $\text{C}=\text{N}$. Stretching vibrations of the ring also in agreement with the literature values (Arieh 2008, Goel et al 1986, Guarner et al 2006, Gupta et al 1990 and Szesesniak et al 1985).

The 1370 cm^{-1} Raman line of pyrimidine corresponding to the vibration ν_{14} has been identified at 1320 cm^{-1} in infrared spectra and at 1295 cm^{-1} in Raman spectra of the said molecule. Goel et al (1986) assigned this mode at 1305 cm^{-1} in the infrared spectra of 2-amino-4-chloro-6-methyl pyrimidine. Some other workers (Balachandran et al 2012, Kumar^c et al 2021 and Rao 1963) have assigned this mode at 1314 cm^{-1} in the spectra of 4,6-dihydroxy pyrimidine. The vibration has been identified at 1305 cm^{-1} in pyrimidine-4-

5, -d₂ (Bersani et al 2010, Deep et al 2013, Eihaty et al 1990, Goel et al 1986, Guarner et al 2006, Gupta et al 1990, Hong et al 2004 and Szezesniak et al 1985)

In substituted benzenes the frequency of one of the two ring modes ν_1 and ν_2 reduces to 820 cm⁻¹ while the other remain at 1000 cm⁻¹ in amino methyl pyrimidine and in 5 methyl pyrimidine (Bellamy 1975 and Rao 1963). The modes ν_1 and ν_2 have been identified at 768, 1000 and 820 and 1050 cm⁻¹ respectively. These modes in 2,4,6-triamino pyrimidine (Lord et al 1976) have been assigned at 796 and 990 cm⁻¹ and in 4,6-dihydroxy-2-methyl pyrimidine at 825 and 987 cm⁻¹ (Goel et al 1986, Guarner et al 2006, Gupta et al 1990, Hong et al 2004, Ingold et al 1953, Jacque et al 1970, Sanyal et al 1978 and Szezesniak et al 1985). In view of these the bands at 760 and 940 cm⁻¹ in infrared spectra and at 970, 985 cm⁻¹ in laser Raman spectra of present molecule have been assigned to correspond to ν_1 and ν_{12} modes respectively. Which also agrees with the literature (Anderson et al 2014, Deep et al 2013, Goel et al 1986, Guarner et al 2006, Hong et al 2004 and Jacque et al 1970)

The vibrations γ_4 , ν_{16} and ν_{16b} in pyrimidine (Anderson et al 2014, Braz et al 2021, Chand^b et al 2021, Deep et al 2013, Goel et al 1986, Guarner et al 2006, Gupta et al 1990, Kumar^{a & b} et al 2021, Jacque et al 1970, Yadav^{a & b} et al 1998 and Yadav et al 2000) appearing at 708, 400 and 709 cm⁻¹ in infrared spectra and 345, 445 and 698 cm⁻¹ in laser Raman spectra of the considered molecule have been attributed to the C-C stretching mode. Sanyal et al (1979) and Rao (1963) assigned these modes at 340, 412, and 695 cm⁻¹ in substituted hydroxy methyl pyrimidine. Some workers (Chand^b et al 2021, Deep et al 2013, Eihaty et al 1990, Kumar^{a & b} et al 2021, Jacque et al 1970, Yadav^{a & b} et al 1998 and Yadav et al 2000) assigned these modes at 335, 400 and 810 cm⁻¹ in the vibrational spectra of substituted chloro methyl mercapto pyrimidine.

The ring planar deformation β_{6a} and β_{6b} in methyl pyrimidine (Anderson et al 2014, Bellamy 1975, Chand^b et al 2021, Gupta et al 1990, Hong et al 2005, Kumar 2000, Kumar^{a & b} et al 2021, Jacque et al 1970 and Szezesniak et al 1985, Yadav^{a & b} et al 1998 and Yadav et al 2000) have been assigned at 559 and 639 cm⁻¹ respectively. Some workers (Bersani et al 2010 and Rao 1963) assigned these modes at 510 and 591 cm⁻¹ in case of substituted hydroxy pyrimidine and also observed at 575 and 610 cm⁻¹ in infrared and laser Raman spectra of substituted pyrimidine (Goel et al 1986, Guarner et al 2006, Gupta et al 1990, Jacque et al 1970, Rao 1963, Szezesniak et al 1985 and Yadav et al

2000). In view of the above the bands observed at 588 and 610 cm^{-1} in infrared spectra and at 570 and 625 cm^{-1} in Raman spectra of present molecule respectively have been contributed to this mode in agreement with the work of other workers (Bersani et al 2010, Bellamy 1975, Chand^b et al 2021, Deep et al 2013, Eihaty et al 1990 and Yadav^{a & b} et al 1998).

C—X Vibrations:

Some workers (Kumar 2000) suggested the occurrence of the C-OH stretching vibrations near 1300 cm^{-1} . Bellamy (1975) and Bersani et al (2010) suggested the C-OH plane bending mode at lower frequency 1200 cm^{-1} . Other workers (Bersani et al 2010, Bellamy 1975, Guarner et al 2006, Gupta et al 1990, Hong et al 2005, Kumar 2000, Kumar^{a & b} et al 2021, Rao 1963, Yadav^{a & b} et al 1998 and Yadav et al 2000) have assigned higher frequency to C-OH stretching mode. The X = Sensitive Vibrations ν_{13} due to C-OH stretching have been identified 1235 and 1260 cm^{-1} in infrared and laser Raman spectra of the said molecule. While the C-OH in plane bending mode ν_{6a} have been identified at 570 and 566 cm^{-1} in infrared and laser Raman spectra.

The C-OH out of plane and O-H torsional mode in in phenol at 244 and 309 cm^{-1} respectively have been assigned by many workers (Junghare et al 2002 and Kim et al 2008). Siquenza et al (1981) have reported the occurrence of O-H torsion around 400 cm^{-1} . So, in view of these the out of plane bending mode γ_5 have been identified at 330 and 326 cm^{-1} in their infrared and laser Raman spectra respectively. The above-mentioned work agrees with the assignments proposed by many workers (Bersani et al 2010, Chand^b et al 2021, Guarner et al 2006, Gupta et al 1990, Hong et al 2005, Jacque et al 1970, Kumar 2000, Kumar^{a & b} et al 2021, Yadav^{a & b} et al 1998 and Yadav et al 2000)

Stretching vibrations ν_2 and ν_{7b} in substituted anilines (Yadav 1992) appear at 1300 cm^{-1} . Goel et al (1986) assigned this mode at 1320 cm^{-1} 1319 and 1330 cm^{-1} in different amino methyl pyridines.

Sanyal et al (1979) assigned the C—NH₂ stretching mode ν_2 at 1244 cm^{-1} in 2,4,6-triamino pyrimidine. Carmona et al (1993) and Kumar^b et al (2021) suggested this band in the region 1250-1340 cm^{-1} in nearly at the primary aromatic amines. The experimental molecule 4,6,2-DAHP contains two NH₂ groups, in view of the above assignments this bands at 1338 cm^{-1} and at 1350, 1385 cm^{-1} have been assigned to ν_2 and ν_7 modes respectively supported by the workers (Anderson et al 2014, Bellamy 1975, Bersani et al

2010, Chand^b et al 2021, Deep et al 2013, Eihaty et al 1990, Gupta et al 1990, Hong et al 2005, Kumar 2000 and Kumar^{a & b} et al 2021). The X-sensitive C—NH₂ in plane bending mode β_{15} and β_{18b} at 385 cm⁻¹ in 3 fluoro-4-Chloro-aniline has been assigned by Sanyal et al (1979).

Mohan (1992) assigned the C—NH₂ in plane bending and out of plane bending mode at 411 and 325 cm⁻¹ in laser Raman spectra of 2-amino pyrimidine molecule. In view of the above the bands at 345 cm⁻¹ in infrared and at 360 cm⁻¹ in laser Raman spectra have been assigned to β_{18b} and β_{15} modes respectively.

The out of plane C—NH₂ modes γ_{10b} and γ_{17a} are also X-sensitive in the infrared and laser Raman spectra of the said molecule. Evans (2008) assigned the C—NH₂ out of plane bending mode at 233 cm⁻¹ in aniline and Green et al (1971) assigned the C—NH₂ out of plane mode at still lower frequency. In the case of said molecule, laser Raman bands at 235 and 250 cm⁻¹ are observed as C—NH₂ out of plane bending modes γ_{17a} and γ_{10b} . This work is in agreement with the results of other workers (Anderson et al 2014, Bersani et al 2010, Guarner et al 2006, Kumar^{a & b} et al 2021, Krishnakumar et al 2012, Yadav^{a & b} et al 1998 and Yadav et al 2000).

OH GROUP VIBRATIONS:

Workers (Bellamy 1975, Bersani et al 2010, Chand^b et al 2021, Deep et al 2013, Hong et al 2005, Kumar^{a & b} et al 2021, Krishnakumar et al 2012 and Yadav et al 2000) suggested that in the molecules containing OH group the -OH valence vibration appears in the range 3500-3700 cm⁻¹. Evans (2008) assigned this mode to the band at 3628 cm⁻¹ in phenol. Sanyal et al (1979) assigned the OH stretching mode at 3705 and 3680 cm⁻¹ in hydroxy pyrimidine. Gupta et al (1986) have also assigned the same mode at 3430 cm⁻¹ 4-amino-5-hydroxy-2-mercapto-pyrimidine.

In the said molecule 4,6,2-DAHP, this mode has been assigned at 3662 and 3624 cm⁻¹ in their infrared and laser Raman spectrum. These may be some interaction between C-OH stretching and O-H in-plane bending vibrations but the lower frequency has been attributed mainly due to the O-H deformation mode. Bersani et al (2010), Bellamy (1975) and Rao (1963) reported a band at 1180 cm⁻¹ possessing strong (O—H) character. Green et al (1977) assigned these bands at 1178, 1189, 1180 cm⁻¹ to this mode in dichloro-phenols.

In view of the above the bands observed at 1145 cm^{-1} in infrared spectra and at 1160 cm^{-1} in laser Raman spectra have been assigned to OH in plane bending mode for the present molecule supported by the work of Vibha et al (1994) and other workers (Kumar^{a & b} et al 2021, Rao 1963, Szczesniak et al 1985, Yadav^{a & b} et al 1998 and Yadav et al 2000). Green et al (1977) assigned the out of plane bending mode at 400 , 366 and 312 cm^{-1} in three dichlorophenols. Sanyal et al (1978) and Bellamy (1975) have assigned OH out of plane bending mode at 345 and 355 cm^{-1} in case of 4,6-dihydroxy-2-methyl pyrimidine.

In view of these assignments the bands at 385 cm^{-1} in the infrared spectra and at 380 cm^{-1} in laser Raman spectra are observed and assigned to OH-out of plane bending mode for present molecule. The work is in agreement with the workers (Anderson et al 2014, Bersani et al 2010, Chand^b et al 2021, Deep et al 2013, Hong et al 2005, Kumar 2000, Kumar^{a & b} et al 2021, Szczesniak et al 1985, Yadav^{a & b} et al 1998 and Yadav et al 2000).

-NH₂ GROUP VIBRATIONS:

Some workers (Bellamy 1975, Bersani et al 2010, Guarner et al 2006, Gupta et al 1990, Huang et al 2020, Kumar 2000, Kumar^{a & b} et al 2021 and Yadav et al 2000) suggests that in primary aromatic amines two bands occur in the region 3300 to 3550 cm^{-1} associated with N-H stretching vibrations. According to Bellamy (1975) in N-octa amide in chloroform solution, the NH₂ free absorption occur at 3530 cm^{-1} and 3415 cm^{-1} . There are also additional bands at 3498 , 3345 , 3300 and 3182 cm^{-1} . In solid state the pattern simplifiers and gives two broader N-H peaks near 3350 cm^{-1} and 3164 cm^{-1} . In view of these the bands observed at 3582 , 3405 , 3330 and 3245 in the infrared and at 3556 , 3434 , 3305 and 3260 cm^{-1} in laser Raman spectrum of the said molecule 4,6,2-DAHP have been attributed to N-H asymmetric and symmetric stretching vibrations. The work has been supported by the work of Sanyal et al (1989) in case of amino substituted pyrimidines.

Another band at 1685 cm^{-1} and 1690 cm^{-1} in infrared and laser Raman spectrum of present molecule have been identified in $\text{C}=\text{O}$ region corresponding to $\text{C}=\text{O}$ stretching. Out of plane modes have also been identified at 550 , 395 cm^{-1} in infrared and at 560 and 400 cm^{-1} in laser Raman spectrum of present molecule in agreement with literature value. This shows that the tautomerism is due to OH group at 2nd position. Although O-H stretching and bending vibrations also appear yet the existence of tautomerism may be taken very weak. Bersani et al (2010), Bellamy (1975) and Rao (1963) suggested that scissoring mode lies in the region 1590 - 1650 cm^{-1} . Because of two -NH₂ groups, there are two -NH₂ scissoring modes identified at 1650 and 1675 cm^{-1} in the infrared spectra and at 1655 and

1660 cm^{-1} in the laser Raman spectrum of present molecule supported from literature (Anderson et al 2014, Bellamy 1975, Bersani et al 2010, Chand^b et al 2021, Deep et al 2013, Eihaty et al 1990, Gupta et al 1990, Hong et al 2005, Yadav^a & ^b et al 1998 and Yadav et al 2000). Evans (2008) has suggested the NH_2 twisting frequency around 1060 cm^{-1} . In the said molecule (4,6,2-DAHP) the interaction of similar frequencies is possible due to two NH_2 groups and this results in the modification of these modes. The strong bands are observed at 1055 and 1105 cm^{-1} in infrared spectrum and at 1035 and 1100 cm^{-1} in laser Raman spectrum of the present molecule, supported from the literature (Anderson et al 2014, Bersani et al 2010, Chand^b et al 2021, Deep et al 2013, Guarner et al 2006, Gupta et al 1990, Hong et al 2005, Kumar 2000, Kumar^a & ^b et al 2021, Yadav^a & ^b et al 1998 and Yadav et al 2000). Evans (1988) and Goel et al (1988) identified the NH_2 wagging vibrations at 670 cm^{-1} and at 655 cm^{-1} respectively. Thus, the bands are obtained at 645 and 655 cm^{-1} and at 640 and 685 cm^{-1} in infrared and laser Raman spectrum of the present molecule 4, 6, 2 DAHP.

Mohan et al (1994) assigned the NH_2 torsion mode at 196 cm^{-1} in substituted amino pyrimidine. But this mode is not identified in infrared spectrum but identified in the laser Raman spectrum at 195 cm^{-1} for the present molecule. The work is supported by many workers (Bellamy 1975, Bersani et al 2010, Chand^b et al 2021, Deep et al 2013, Goel et al 1988, Gupta et al 1990, Hong et al 2005, Jacque et al 1970 and Kumar 2000).

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