

Laser Raman and Infrared Spectra of Amino Hydroxy Pyrimidine

Dr. Ajay Kumar

Assistant Professor, SKD University, Hanumangarh (Raj.)

ajaaykumar187@gmail.com

Abstract:

This Paper Comprises Of The Investigations On The Infrared And Laser Raman Spectra Of 2,5-diamino-4,6-dihydroxy Pyrimidine. The Infrared Spectra Is Recorded In The Region 200 – 4000 cm^{-1} Using KBr Pallet Technique. Laser Raman Spectra is Recorded In The Region 100 – 4000 cm^{-1} . The Observed Vibrational Frequencies Are Assigned To Different Modes Of Vibrations By Considering C_{2v} Point Group Symmetry. On The Basis Of Magnitude And Relative Intensity Of The Recorded Spectra And Group Symmetry Approach With Analogy To The Similar Molecules.

Introduction:

Amongst in the N-heterocyclic molecules, the pyrimidine when substituted with hydroxy (OH), methyl (CH_3) and amine (NH_2) gives us biological important molecule like cytosine, thymine and uracil etc. The investigations of substituted pyrimidine draw considerable attention because of significant role of N-heterocyclic molecule into the structural problems of nucleic acid. In these molecules, the role of substituent plays a very significant role. As on dated, some detailed spectroscopic studies have been reported in the literature value for pyrimidine [1,2], substituted pyrimidine [3-6] and nuclei acid constituent [7-10]. Because of low symmetry and limited information about the molecular parameters, reliable theoretical calculations for these molecules is impossible. So, it was considered to understand the role of substituents through experimental techniques. It has been possible to have tautomeric structures with substituents like hydroxy group (OH) and amine group (NH_2) as reported in the case of 4,6-dihydroxy pyrimidine and 4,5-diamino pyrimidine respectively by some workers [11]. Jacque and Lebas [12] have reported the vibrational spectra of different substituted pyrimidines. Some workers [13-25] have reported the vibrational spectra of substituted pyrimidines and their analogous molecules. The absorption spectra of uracil and cytosine nucleosides have been well predicted on theoretical ground by Berthod et al [26]. In view of this, the present article reports the study of Laser Raman spectra, Infrared spectra and Complete vibrational analysis of observed frequencies of 2,5-diamino-4,6-dihydroxy pyrimidine.

Experimental Details:

Spectroscopic grade sample of 2,5-diamino-4,6-dihydroxy pyrimidine (hereafter referred as 2,5,4,6-DADHP) have been taken. A few milligrams of this sample was mixed with the KBr of spectroscopic grade and passed into the disc. Finally pallets of the sample have been formed. The infrared spectra was recorded in the region 200-4000 cm^{-1} on Perkin Elmer spectrophotometer. The laser Raman spectra was recorded by using 488 nm line of Ar^+ for the excitation in the region 200-4000 cm^{-1} on a Carry Model - 82 grating spectrophotometer through a 4 W Argon laser.

Result and Discussion :

The molecular structural formula of the compound 2,5,4,6-DADHP is shown in Figure 1.

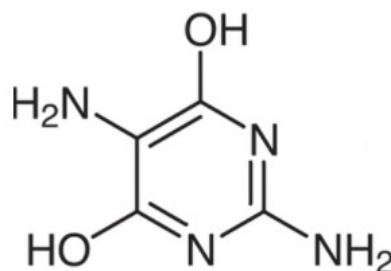


FIGURE: 1 MOLECULAR STRUCTURE OF 2,5,4,6-DADHP

The structure of several pyrimidine compounds have been determined by some workers [4,5] and in all such cases, the molecules were found to be planar. The observed fundamental vibrational frequencies present in the infrared and laser Raman spectrum are shown in Table-1. The amino group frequencies along with their correlation with similar molecules are shown in Table-2. The hydroxy (OH) group frequencies along with their correlation to similar molecules are shown in Table-3. All the fundamental frequencies are have been described in the form of Wilson's notations and have also been compared with the mode of pyrimidine-2 [1] as shown in Table-1. From the point of view of the position of the substituents and by considering amine (NH₂) group as a single mass point, the said molecule would have C_{2v} point group symmetry.

Vibrational Spectra :

Ring Vibrations:

The ring stretching vibrations are very much prominent in the spectrum of benzene and their derivatives. They are highly characteristic of the aromatic ring itself. In the spectrum of pyrimidine, there are three C-H stretching belonging to the b₂ species. When it is substituted at fourth and sixth position, the modes ν_{13} and ν_{7b} are dropped which are in accordance with the assignments specified by Nehad and Stidham [1]. Bellamy, Rao and Varsanyi [27-29] suggested that if the molecule is completely substituted, no C-H stretching vibration is expected that lies in the region 3100 – 3000 cm⁻¹. On the other hand, no band are observed corresponding to C-H in-plane bending mode and C-H out-of-plane bending mode in the infrared and Raman spectra of the said molecule. The spectra of pyrimidine indicate these modes at 811, 1225 and 3074 cm⁻¹. S Mohan and V Illangovan [30] have also shown these modes at 825, 1177 and 3018 cm⁻¹ in case of 2-amino pyrimidine.

The spectra of pyrimidine have shown the pairs of absorption bands at 1398 (ν_{19a}), 1466 (ν_{19b}), 1564 (ν_{8a}) and 1568 (ν_{8b}) cm⁻¹ which are analogous to the pair of bands originating from e_{1u} (1485) and e_{2g} (1995) modes of benzene and also found in substituted pyrimidine [27].

The modes ν_{1g} is basically a ring deformation and involves both stretching and bending mode of carbon bonds while the bands at ν_8 consists of lateral dilation and contraction of the ring produced mainly through stretching and compressing of the bands as specified by Rao and Varsanyi [28,29]. The mode ν_{19a} was found at 1382 cm⁻¹ in 2-chloro pyrimidine [31] and at 1391 cm⁻¹ in 5-methyl pyrimidine [5]. In view of these assignments, in the present study the modes at ν_{19a} , ν_{19b} , ν_{8a} , and ν_{8b} are found at 1350/1320, 1396/1380, 1448/1430, 1500/1480 and 1550/ 1520 cm⁻¹ respectively. These bands in analogy with the spectra of substituted benzenes are because of double bond C=C and C=N stretching vibrations of the benzene ring.

Sanyal et al [25] have also assigned such modes at 1430, 1550, 1464 and 1581 cm⁻¹ in the 2,4,6-triamino pyrimidine. Also, these bands are found at 1585, 1385, 1485 and 1617 cm⁻¹ in case of 4,6-

dihydroxy-2-methyl pyrimidine. These assignments also find support from the literature value [6,7]. The mode ν_{14} corresponding to 1370 cm^{-1} Raman line of pyrimidine have been identified at 1350 and 1320 cm^{-1} in infrared and Raman spectra of the said compound 2,5,4,6-DADHP. This mode has been identified at 1315 and 1335 cm^{-1} in infrared and Raman spectra of 6-amino-2-methyl pyrimidine [32] which is very close to the corresponding mode of the present molecule.

In substituted benzenes, the frequency of one of the two ring modes ν_1 and ν_{12} reduces to 820 cm^{-1} while the other found at 1000 cm^{-1} . Ingold [33], suggested that the energy corresponding to carbon stretching (ring breathing) vibration a_{1g} (995 cm^{-1}) and carbon planar bending vibration b_{1u} (1010 cm^{-1}) modes of benzene are very close to each other. Therefore, there will be an appreciable interaction between the two and as a result the energies of two vibrations will be modified.

It has been observed that the ring stretching vibration reduces to a large amount depending upon the mass, nature and number of substituents while the bending remains very close to 1010 cm^{-1} . Secondly, the vibration corresponding to a_{1g} (995 cm^{-1}) is completely symmetric, which appears as a polarized and intense band in the Raman spectra. The ν_1 and ν_{12} modes are observed at 768 and 1000 cm^{-1} in 5-methyl pyrimidine [5]. Hence, in view of these assignments, the bands at 730 , 750 , 800 and 790 cm^{-1} in infrared and Raman spectra of the title molecule have been assigned correspond to ν_1 and ν_{12} modes respectively. These values find support from the literature value as specified by Sanyal et al [25], Goel et al [14-18] and others [34,35].

The ring out-of-plane bending vibrations ν_4 , ν_{16a} and ν_{15b} in pyrimidine appears at 708 , 399 and 344 cm^{-1} respectively. The bands observed at 620 , 305 and 330 cm^{-1} in infrared spectra and at 600 , 310 and 290 cm^{-1} in Raman spectra of the said compound 2,5,4,6-DADHP have been assigned to these modes respectively. These assignments find support from the literature value of Goel et al [21-24] and Job & Kartha [5] in substituted pyrimidines.

The ring planar deformation ν_{6a} and ν_{6b} in the compound 5-methyl pyrimidine were assigned at 559 and 639 cm^{-1} respectively. In the present molecule, these modes are identified at 500 and 490 cm^{-1} in their respective infrared and Raman spectra. Goel et al [20] have assigned all these modes at 780 , 610 , 400 , 420 and 1305 cm^{-1} in the molecule 2-amino-4-chloro-6-methyl pyrimidine. It shows good correlation with these assignments of the present molecule. Also Goel et al [16] have assigned these modes at 335 , 410 , 455 , 562 , 768 and 1000 cm^{-1} in case of 2-amino-4-methyl pyrimidine. In case of 5-methyl cytosine, these modes are specified at 410 , 445 , 610 , 660 , 976 and 1018 cm^{-1} . All these assignments are in agreement with the work observed by several workers [8-10,25,30].

C-X Vibrations:

Kletz et al [35] have suggested the occurrence of the C-OH stretching vibration near 1300 cm^{-1} , while Bellamy [27] suggested that the C-OH in-plane bending mode lies at lower frequency near 1200 cm^{-1} . Hadzi et al [26] have assigned the higher frequency to C-OH stretching mode. The X-sensitive vibration ν_{13} due to C-OH stretching (OH at 5th and 6th position) have been identified at 1290 , 1280 and 1310 , 1300 cm^{-1} in infrared and Raman spectra of said molecule. While the C-OH in-plane bending mode ν_{9a} have been identified at 580 , 560 and 600 , 590 cm^{-1} in infrared and Raman spectra.

Bist et al [36] assigned the C-OH out-of-plane bending mode and O-H torsional mode in phenol at 244 and 309 cm^{-1} respectively. Siquenza et al [37] have reported occurrence of O-H torsion around 400 cm^{-1} . In view of these assignments, out-of-plane bending mode ν_5 have been identified at 370 , 380 , 400 , 410 , 290 and 260 cm^{-1} in the infrared and laser Raman spectra respectively. These assignments are also in agreement with the literature value [4,5,18].

In substituted anilines [18], the C-NH₂ stretching vibrations ν_1 and ν_{7b} appears near 1300 cm^{-1} . Goel et al [14] have assigned this mode at 1320 , 1319 and 1330 cm^{-1} in different amino methyl

pyridines. Some workers [38,39] have assigned the C-NH₂ stretching vibrations ν_2 at 1244 cm⁻¹ in 2,4,6-triamino pyrimidine. Carmona et al [40] have also suggested this band in the region 1250-1340 cm⁻¹ in nearly at the primary aromatic amines. The present molecule contains two amine group, so in view of these assignments the bands observed at 1410, 1400 cm⁻¹ and at 1480, 1450 cm⁻¹ have been assigned to ν_2 and ν_{7b} modes respectively. These assignments also find support from the literature value [24,25].

Sanyal et al [25] have assigned the X sensitive C-NH₂ in-plane bending mode ν_{15} and ν_{18b} at 385 cm⁻¹ in 3-fluoro-4-chloro aniline. S Mohan [30] have assigned the C-NH₂ in-plane bending mode and out-of-plane bending mode at 411 and 325 cm⁻¹ in laser Raman spectra in 2-amino pyrimidine. Therefore, in view of these assignments, the bands at 350 cm⁻¹ in infrared and at 345 cm⁻¹ in laser Raman spectra have been assigned to ν_{18b} and ν_{15} modes respectively. The out-of-plane mode ν_{10b} and ν_{17a} are also X-sensitive in the infrared and laser Raman spectra of the title molecule. Evans [41] has assigned the C-NH₂ out-of-plane bending mode at 233 cm⁻¹ in aniline. Green et al [42] have assigned this mode at still lower frequency. In the present case, only laser Raman bands at 290 and 260 cm⁻¹ are assigned as C-NH₂ out-of-plane bending mode ν_{17a} and ν_{10b} . These assignments are in agreement with the results observed by some workers [3-5,18,30].

Group Vibrations :

-OH Groups:

Some workers [16,17] have suggested for molecules containing hydroxy groups, the O-H valance vibration appears in the range 3500-3700 cm⁻¹. Evans [41] assigned this mode at 3628 cm⁻¹ in phenol. Sanyal et al [25] assigned O-H stretching mode at 3705 and 3680 cm⁻¹ in 4,6-dimethyl pyrimidine. Some workers [24,43] have also assigned this mode at 3430 cm⁻¹ in 4-amino-6-hydroxy-2-mercapto pyrimidine.

In the present molecule 2,5,4,6-DADHP, this mode have been found at 3650, 3600, 3700 and 3650 cm⁻¹ in their infrared and laser Raman spectra. There is some possibility of interaction between C-OH stretching and O-H in-plane bending vibrations. But in these assignments, the lower frequency is attributed mainly due to the O-H deformation mode. Mecke et al [44] have assigned a band at 1180 cm⁻¹ which possesses a strong O-H character. Green [42] have assigned this band at 1178, 1189 and 1180 cm⁻¹ in case of 2,6-dichloro, 2,5-dichloro and 3,4-dichloro phenols respectively.

In view of these assignments, the bands observed at 1200, 1260, 1190 and 1240 cm⁻¹ in infrared spectra and at 1156 cm⁻¹ in laser Raman spectra are assigned to O-H in-plane bending mode for the molecule 2,5,4,6-DADHP. It find support from the literature value [30]. Some workers [45] have assigned the O-H 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 350 cm⁻¹ in the infrared spectra and at 345 cm⁻¹ in laser Raman spectra are assigned to O-H out-of-plane bending mode for the molecule 2,5,4,6-DADHP. It also find support from the literature value [45].

NH₂ Group:

Many workers [16,17] suggested that in most of the primary aromatic amines, there occur two bands in the region 3350-3550 cm⁻¹ which are associated with N-H stretching vibrations. It has been assigned by Bellamy [27] that in case of N-octa-amide in chloroform solution, the NH₂ free absorption occur at 3530 cm⁻¹ and 3415 cm⁻¹, but it also indicates additional bands at 3498, 3345, 3300 and 3182 cm⁻¹. This type of simultaneous association of free and bonded N-H bonds. In solid states, the pattern simplifies and gives two broader N-H peaks near 3350 cm⁻¹ and 3164 cm⁻¹. In view of these assignments, the bands observed at 3150, 3300, 3450 and 3500 cm⁻¹ in infrared spectra and bands at 3190, 3290, 3390 and 3500

cm^{-1} in laser Raman spectra of the present molecule 2,5,4,6-DADHP have been assigned to N-H asymmetric and symmetric stretching vibrations respectively. These assignments also find support from the literature value [4,19] in different amino substituted pyrimidines.

The bands observed at 1700, 1690 cm^{-1} in the infrared spectra and 1800, 1750 cm^{-1} in the laser Raman spectra of said molecule 2,5,4,6-DADHP are assigned to C=O stretching while the band identified at 350, 290 cm^{-1} in infrared spectra and bands observed at 260, 345 cm^{-1} in laser Raman of the said molecule 2,5,4,6-DADHP are assigned to out-of-plane modes. Both these bands find support from the literature value [28]. This shows that the tautomerism is because of OH group. However, when the O-H stretching and bending vibrations also appears, the existence of tautomerism may be taken to be very weak.

Some workers [16,17,26] suggested that scissoring mode lie in the region 1590-1650 cm^{-1} . Because of two NH_2 group, it has been observed two NH_2 scissoring mode at 1650 & 1580 cm^{-1} in the infrared spectra and 1620 & 1500 cm^{-1} in laser Raman spectra of the said molecule 2,5,4,6-DADHP. These assignments find support from the literature value [26]. Evans [41] has suggested the NH_2 twisting frequency near 1060 cm^{-1} . In 2,5,4,6-DADHP, due to two NH_2 group, the interaction of similar frequencies is possible that may modify these modes. Hence the strong bands observed at 1050 and 1140 cm^{-1} in the infrared spectra and at 1040 and 1120 cm^{-1} in laser Raman spectra of the present molecule 2,5,4,6-DADHP. These assignments also find support from the literature value [45].

The NH_2 wagging vibration has been identified at 670 cm^{-1} by Evans [41]. Whereas Goel et al [15] have assigned this band at 655 cm^{-1} . In view of these assignments, the bands observed at 650 cm^{-1} in infrared spectra and at 660 & 680 cm^{-1} in laser Raman spectra in the molecule 2,5,4,6-DADHP have been assigned to NH_2 wagging mode. Mohan et al [30] have assigned the NH_2 torsion mode at 196 cm^{-1} in 2-amino pyrimidine. In the present study, this mode has been identified at 250 cm^{-1} in the infrared spectra and at 200 cm^{-1} in laser Raman spectra. This assignment also find support from the literature value [14-17,25,39].

Table - 1

Assignment of Vibrational Frequencies in (cm^{-1}) of 2,5,4,6-DADHP

2,5-Diamino-4,6-Dihydroxy Pyrimidine		Pyrimidine	Assignments
IR	Laser Raman		
200 vvw	180 vvw	-	γ (C-NH ₂)
210 vvw	200 vvw	-	NH ₂ torsion
250 vvw	225 vw	-	(O-H) torsion
290 vvw	260 vvw	-	γ (C-NH ₂), γ (O-H)
305 vw	290 vw	-	γ (C=O)
330 vw	310 vvw	-	γ (C=O)
350 vw	345 w	-	γ (C-NH ₂), γ (O-H)
370 w	380 vs	-	γ (C-OH)
400 w	410 w	-	γ (C-OH)
500 vs	490 s	-	β (C=O)
540 s	520 vs	-	β (C=O)
580 w	560 w	-	β (C-OH)
600 vs	590 vs	-	β (C-OH)
620 vw	600 vw	-	β (C-C)
650 vw	660 vw	-	NH ₂ wagging
680 s	690 s	-	NH ₂ wagging
750 vvs	730 vvs	650	γ (C-C) (C-N)
800 vs	790 vs	678	γ (C-C) (C-N)
900 w	850 vw	992	γ (C-C) (C-N)
1000 vvs	990 vs	925	β (C-C) (C-N)

1050 s	1040 s	-	NH ₂ twisting
1100 vs	1090 vs	-	β (C-NH ₂)
1140 vvw	1120 vvw	-	NH ₂ twisting
1180 vw	1160 vw	-	β (C-NH ₂)
1200 vs	1190 s	-	β (O-H)
1260 vs	1240 s	-	β (O-H)
1290 vs	1280 s	-	ν (C-OH)
1310 w	1300 w	-	ν (C-OH)
1350 w	1320 vw	1350	ν (C-C)
1390 w	1380 vw	1370	ν (C-C)
1410 vvw	1400 vvw	-	ν (C-NH ₂)
1448 vw	1430 vvw	1466	ν (C-C)
1480 vw	1450 w	-	ν (C-NH ₂)
1500 w	1480 w	1564	ν (C-C)
1550 s	1520 s	1568	ν (C-C)
1580 w	1560 w	-	NH ₂ Scissoring
1650 vs	1620 s	-	NH ₂ Scissoring
1720 s	1690 w	-	ν (C=O)
1800 w	1750 s	-	ν (C=O)
3150 s	3190 vs	-	ν (NH Asymmetric)
3300 s	3290 w	-	ν (NH Asymmetric)
3450 w	3390 w	-	ν (NH Symmetric)
3500 w	3480 w	-	ν (NH Symmetric)
3650 w	3600 w	-	ν (O-H)
3700 w	3650 w	-	ν (O-H)
3730 vw	3680 vw	-	ν (N-H)
3790 vw	3710 vw	-	ν (N-H)

Where ν = stretching, β = in-plane bending, γ = out-of-plane bending, w = weak, vw = very weak, vvw = very very weak, s = strong, vs = very strong, vvs = very very strong

Table 2
Comparison of amino group frequencies with identical molecules

2,5,4,6-DADHP		2-AP	2,4,6-TAI	Assignments
IR	Raman			
250	200	197	-	NH ₂ torsion
650	660	670	648	NH ₂ wagging
-	680	-	-	NH ₂ wagging
1140	1120	1130	1094	NH ₂ twisting
1050	1040	-	-	NH ₂ twisting
1580	1500	-	-	NH ₂ scissoring
1650	1620	1647	1642	NH ₂ scissoring
3150	3190	-	-	ν (N-H) asym
3300	3290	3375	3319	ν (N-H) asym
3400	3390	-	3430	ν (N-H) symm
3500	3480	3555	-	ν (N-H) symm

(All values are in cm^{-1})

Where ν =stretching, symm = symmetric, asymm = asymmetric,

2,5,4,6-DADHP = 2,5-diamino-4,6-dihydroxy pyrimidine

2-AP = 2-amino pyrimidine

2,4,6-TAP = 2,4,6-5-triamino pyrimidine

Table - 3
Comparison of hydroxy group frequencies with identical molecules (All values are in cm^{-1})

2,5,4,6-DADHP		4,6,2-DMHP		2,4,6-DAHP		Assignments
IR	Raman	IR	Raman	IR	Raman	
3700	3650	3600	3670	3660	3620	ν (O-H)
3650	3600	-	-	-	-	
1260	1240	1315	1305	-	-	β (N-H)
1200	1190	-	-	-	-	
350	345	305	295	380	375	ν (N-H)
290	260	-	-	-	-	
250	225	-	-	-	-	(O-H) torsion

Where ν = stretching, β = in-plane bending, γ = out-of-plane bending

2,5,4,6-DADHP = 2,5-diamino-4,6-dihydroxy pyrimidine

4,6,2-DMHP = 4,6-dimethyl-2-hydroxy pyrimidine

2,4,6-DAHP = 2,4-diamino-6-hydroxy pyrimidine

REFERENCES

- 1) F.M. Nehad and H.Q. Stidham, *Spectrochim Acta*, **13A**(1975)1433.
- 2) T. Shimanouchi, M. Tsuboi and Y. Kyogobu, "Advances in Chemical Physics", New York, **7** (1964)435.
- 3) M.T. Ei-Haty, A.E. Mohamed, F.A. Adam and A. A. Gabr, *Spectrochim Acta*, **46A**(1990)1743.
- 4) Wheatley, *Acta Crystallogr*,**13**(1960)80.
- 5) V.A. Job and S.B. Kartha, *Indian Acad. Sci.*,**85A** (1977)476.
- 6) L.B. Sebagh and J. Zavemhowitch, *Spectrochim Acta*, **32**(1976)797.
- 7) T.U. Ogeta, H. Shimada and R. Shimade, *Bull. Chem. Soc.*, **57**(1984) 3300.
- 8) J. Banadkar and G. Zudel, *Spectrochim Acta*, **39A**(1983)337.
- 9) D.N. Sathanaryana and S.V.K. Raja, *Spectrochim Acta*,**41A**(1985)804.
- 10) M.K.Yadav, Ph.D. Thesis, C.C.S. University, Meerut (1999).
- 11) S.L. Srivastava and Rohitashava, *Indian J. Physics*, **27(3)**(1979)29.
- 12) Jacque Lafaix and J.M. Lebas, *Spectrochim. Acta*, **26A**(1970)1243.
- 13) B.S. Yadav, Vipin Kumar and M.K. Yadav, *Indian J Pure & Appl Phys*, **36**(1998)557.
- 14) R.K. Goel and C. Gupta, *J Raman Spectrosc.*, (1985)16.
- 15) R.K. Goel and S.N. Sharma, *Indian J Pure & Appl Phys*, **14** (1976)842.
- 16) R.K. Goel, N.K. Sanyal and S.L. Srivastava, *Indian J Pure & Appl Phys*, **14** (1976)842.
- 17) R.K. Goel and S.N. Sharma, *Indian J Pure & Appl Phys*,**17**(1979)630.
- 18) R.K. Goel, C. Gupta and S.P. Gupta, *Indian J Pure & Appl Phys*,**23**(1985)344.
- 19) R.K. Goel, S.K. Gupta, M.L. Agarwal and S.N. Sharma, *Indian J Pure & Appl Phys*,**50**(1981)419.
- 20) R.K. Goel and S. Ahmad, *Indian J Phys*,**599(B)**(1985)501.
- 21) R.K. Goel, S.K. Gupta, R.M.P. Jaiswal and P.P. Garg, *Indian J Pure & Appl Phys*,**18**(1980) 223.
- 22) R.K. Goel, S.K. Sharma and S.K. Gupta, *Proc. Nat. Conf. Vibr. Spect. (India)* (1981)117.
- 23) R.K. Goel, S.K. Gupta, R.M.P. Jaiswal and P.P. Garg, *Acta Phys. Polon*, **59A**(1981)665.
- 24) R.K. Goel, S.P. Gupta, S. Sharma and C. Gupta, *J. Chem. Soc. Faraday Trans.*, **282**(1986) 123.
- 25) N.K. Sanyal, R.K. Goel, K.P. Kansal and S.N. Sharma, *Indian J Pure & Appl Phys*, **17(12)** (1979)22.
- 26) D. Hadzi and N. Shepard, *Trans Faraday Soc.*, **50**(1954)911.
- 27) L.J. Bellamy, "The Infrared Spectra of Complex Molecules", (Chapman and Hall, London)(1975).
- 28) C.N.R. Rao, "Chemical Applications of Infrared Spectroscopy", (Academic Press, New York)(1963).
- 29) G. Varsanyi, "Assignments for Vibrational Spectra of Benzene Derivatives", (Adam Hilger, London) (1974).
- 30) S. Mohan and V. Illan Govan, *Indian J Pure & Appl Phys*, **32**(1994)91.
- 31) Y.A. Sharma, *Spectrochim Acta*, **30A**(1974)01.
- 32) R.K. Goel, *J. De. Chimie. Physigne*, **9**(1984)81.
- 33) C.K. Ingold, *J. Chem. Soc.*, I-XII (1948).
- 34) Vibha Sharma, S.D. Sharma and B.S. Yadav, *Acta Ciencia Indica*, **XXP(4)** (1994)116.
- 35) T.A. Kletz and N.C. Price, *J. Chem. Soc.*, (1947) 644.
- 36) H.D. Bist, J.C.D. Brand, D.R. Nilliams, *J. Molec. Spectrosc.*, **24**(1967)402.
- 37) C. Siquenza, P.F. Canzalez-Diaz, *J. Mol. Struct.*, **72**(1981)165.
- 38) N.K. Sanyal, S.L. Srivastava and R.K. Goel, *Indian J Pure & Appl Phys*, **16**(1978)719.
- 39) Vipin Kumar and Subhash Chandra, *Wutan Hutan Jisuan Jishu Journal*, **XVII (II)**(2021)357.
- 40) P. Carmona, M. Molina and R. Excobar, *Spectrochim Acta*, **49(A)**(1993)1.
- 41) Evans, *Spectrochim Acta*, **16**(1960)428.
- 42) J.H.S. Green, *J. Chem. Soc.*, (1961)236.
- 43) Vipin Kumar and Subhash Chandra, *Vidyabharati International Interdisciplinary Research Journal*, **Oct** (2021)375.
- 44) Mecke and Rossamy, *J. Electrochim*, **59**(1955) 866.
- 45) E.V. Huded, A.M. Huratikoppi, N.H. Ayachit, M.A. Shashidhar and K. Sanarayana Rao, *Ind. J. Phys.*, **59**(1985)211.