



Spectroscopic study of substituted pyridine, a molecule of biological interest

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ABSTRACT

The pyridine ring system is important structural unit in the natural products and compounds of pharmaceutical interest. Some workers shown that pyridine molecule has planar structure in the ground state and quasi planar in excited state. In the present study the infrared and laser Raman spectra of 4-Cyanopyridine have been recorded. The spectra have been analyzed and assignments to observed fundamentals and the group vibrations have been proposed. During the discussion C_{2v} point group symmetry has been assumed. The correlation of the cyano group frequencies (infrared and laser Raman spectra) have been discussed.

Key words: Infrared spectra, laser Raman spectra

DOI Number: 10.48047/nq.2022.20.22.NQ10038 NeuroQuantology 2022; 20(22):533-548

INTRODUCTION:

The N-heterocyclic molecules like pyridine pyrimidine, cytosine, uracil etc. and their derivatives are of great importance because of their role in the structure and properties of biologically important nucleic acids. The pyridine ring system is important structural unit in the natural products and compounds of pharmaceutical interest (Jesson et al 1972 & Martin 1951). Some workers (Kaya et al 1976 & Kumar^a & ^c et al 2022) shown that pyridine molecule has planar structure in the ground state and quasi planar in

excited state. They reported the systematic study of the electronic absorption and laser Raman spectra. Some more workers (Ahmad et al 1990, Bernhard 1995, Govindarajan et al 2014 and Wilmshurst 1957) tabulated the spectral study of pyridine and also studied the vibrational spectra of biologically important pyridine derivatives. The high complexity and low symmetry of these molecules makes the interpretation quite difficult. Chand et al (2021) have reported the sufficient study regarding pyridine and its derivatives. Several workers (Medhi et



al 1990, Navati 1997 and Rao 1997) have investigated for cyano substituted pyridine and substituted benzoinitriles. It is the basis of this discussion.

The object of the present study is to investigate the IR and Raman frequencies corresponding to the substituents and to study the ring fundamentals and their correlations with similar molecules. Considering the cyano group as a single mass point, the interpretation of the molecules under consideration is made by assuming the C_{2v} point group symmetry.

EXPERIMENTAL:

Spec pure samples of 4-cyanopyridine (known as 4-CP), obtained readymade and have been used as such without further purification. The purity had been confirmed by elemental analysis and melting point determination. The infrared spectra of the said compound were recorded by thin film method in the region $4000-600\text{ cm}^{-1}$ on Perkin Elmer FTIR spectrometer model 1210 and in the region $600-400\text{ cm}^{-1}$ on Perkin Elmer FTIR spectrophotometer model 1710 by thin film method. The laser Raman spectra of the molecule has been recorded in the region $3500-100\text{ cm}^{-1}$ on Bruker IFS 66v model FTIR instrument with necessary accessories by using the art laser source of 200 mw power exciting at 488 nm line. The frequencies of all the sharp bands are accurate to $\pm 1\text{ cm}^{-1}$.

RESULTS AND DISCUSSION:

The molecular structural diagram of the said molecule is shown in figure 1 with classical numbering of atoms. The recorded IR and laser Raman spectra for the given molecule are shown in figure 2 and 3. The observed frequencies and their intensities with probable assignments of the molecule under consideration along with the comparison with similar molecule are given in Table 1. The observed cyano group frequencies of the title molecule and its correlation with similar molecules is given in Table 2. The molecule has 30 vibrations which have been divided into various species as $11a_1 + 10b_2 + 2a_2 + 6b$, According to selection rule, a_2 species is inactive for the molecule in the infrared spectra.

-CN STRETCHING VIBRATION:

The Nitrogen atom of pyridine is isoelectronic with the C-H Group since there is little difference in mass or in the bond strengths to adjacent atoms, therefore it is expected that the majority of the fundamental frequencies will be very close to those of benzene and the difference only will arise due to vibrations which involve collective motions of the hydrogen atoms. Many workers have already shown this phenomenon (Bersani et al 2010, Kline et al 1944, Kroto 1975 and Kumar^{b&d} et al 2022).



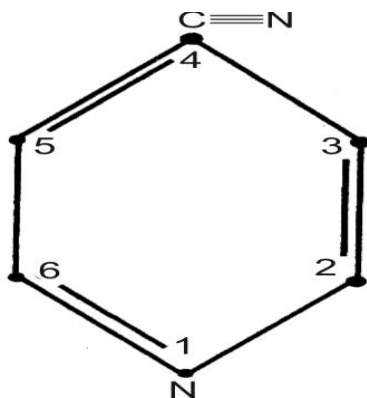


Figure 1: Molecular structure of 4-Cyano Pyridine

The C-H Stretching modes of pyridine are essentially similar to those of Benzene. Bellamy (1975) and other workers (Bersani et al 2010, Garoz et al 2019, Kroto 1975 and Kumar^a & b et al 2021) observed that multiple absorption bands in the vibrational spectra of pyridines in the region 3020-3070 cm^{-1} are due to C-H stretching vibrations. The C-H Stretching frequencies arise from the mode a_{1g} 3062 cm^{-1} e_{2g} 3047 cm^{-1} b_{1u} 3060 cm^{-1} and e_{1u} 3080 cm^{-1} of benzene. So, a strong band at 3068 cm^{-1} and a very weak band at 3005 cm^{-1} in the IR spectra and a weak band at 3090 cm^{-1} and a medium strong band at 3065 cm^{-1} in the Raman spectra for 4-CP are assigned to CH Stretching Vibrations. These are in accordance with the literature value (Bersani et al 2010, Chand et al 2021, Garoz et al 2019, Kroto 1975, Kumar^a & b et al 2021, Medhi et al 1990 and Varsanyi et al 1977).

C-H IN PLANE AND OUT OF PLANE BENDING VIBRATIONS:

There are two degenerate e_{1g} (1178 cm^{-1}) and e_{1u} (1037 cm^{-1}) and two non-degenerate b_{2u} (1152 cm^{-1}) and a_{2g} (1340 cm^{-1}) vibrations involving C-H in plane bending vibrations in the spectra of benzene. In the present work, these modes give four planar bending vibrations involving C-H in plane bending. The frequencies observed at 1246, 1185, 1080 and 1044 cm^{-1} of the medium strong intensities in the infrared spectra and 1290, 1190, 1046, 1044 cm^{-1} of very weak to medium strong intensities in the laser Raman spectra for 4-CP have been assigned to C-H in plane bending vibrations. This is in accordance with the work of researcher (Bersani et al 2010, Chand et al 2021, Garoz et al 2019, Green et al 1977, Kroto 1975, Kumar^a & b et al 2021, Medhi et al 1976, Metha 2012 and Mettler 2018).

The C-H out of plane bending vibration arise from b_{2g} (985 cm^{-1}) e_{1g} (850 cm^{-1}) and a_{2u} modes of benzene and they are expected to occur in the (673 cm^{-1}) region (1000-600 cm^{-1}). According to Bellamy in the case of benzene substitution the strongest band originates in the out of plane bending of the unsubstituted hydrogen atoms of the ring. The principal factor for the frequency is the number of such free hydrogen atoms which are adjacent to one



another. In pyridine derivatives similar effect can be observed. Pyridine with 5 Hydrogen atoms is similar in this region to a monosubstituted benzene also.

The second band appears at lower frequency corresponding to a ring deformation. A similar mode is responsible for 695 cm^{-1} band in monosubstituted derivatives. This band can occur over a wider frequency range. So, the bands at 908 cm^{-1} in infrared and at 780 cm^{-1} in the laser Raman spectra for 4-CP have been assigned as CH out of plane bending Vibrations. This is in accordance with the literature value (Bersani et al 2010, Chand et al 2021, Garoz et al 2019, Kumar^{a & b} et al 2021, Medhi et al 1976, Metha 2012 and Mettler 2018).

RING VIBRATIONS:

C-C, C-N, STRETCHING VIBRATIONS OF PYRIDINE:

According to Bellamy (1975) and Rao (1963) have four ring stretching vibrations in the region $1610\text{-}1400\text{ cm}^{-1}$ and is similar to that of benzene. The highest frequency band of the group occurs between $1615\text{-}1585\text{ cm}^{-1}$ with occasional lower value on heavy substituents. Nature and position of the substituents matters small. In, mono substituted derivatives the frequency occurs in the region 1615 to 1585 cm^{-1} depending upon the nature of substituent changing from electron donor to and electron acceptor.

The benzene double degenerate mode e_{2g} 1595 cm^{-1} consist of lateral dilation and contradiction of the bands and is separated in to two modes after the removal of degeneracy. The first mode is insensitive towards the substituent. In the case of title molecule, it has been found at 1583 cm^{-1} in the laser Raman spectra for 4-CP. The second mode is identified in the region $1536\text{-}1614\text{ cm}^{-1}$. Varsanyi (1977) and is more sensitive towards the substituent. This mode is detected only in infrared spectra at 1563 cm^{-1} for 4-CP. These modes have been assigned to C-C stretching and it is in accordance with the literature value (Bersani et al 2010, Dyer 1965, Kumar et al 2022, Navati et al 1997, Rao 1963 and Sajan et al 2004).

Characteristic aromatic ring vibrations appear in the region $(1600\text{-}1350)\text{ cm}^{-1}$ in almost all heterocyclic compounds Rao (1963). Nature of the ring and type of substituent determines the position and intensity of these vibrations. The six membered heterocyclic ring shows four bands around 1605, 1575, 1480 and 1430 cm^{-1} . These bands become intense when the substituents are electron acceptor in nature because they can conjugate better with the ring. The aromatic conjugation lowers the ring stretching frequency.

In the conjugated nitrogen containing ring system like pyridine and similar



aromatic compounds the individuality of the ring CN absorption is completely lost. It also finds support from the literature value (Bellamy 1975, Bersani et al 2010 and Rao 1963).

The characteristic patterns of absorption of the ring stretching vibrations of 5 and 6 membered rings results from the complete interaction of the CC and CN vibrations and it is therefore difficult to isolate the different vibrations.

In the 4-substituted pyridines (Bersani et al 2010 and Kartrizky 1959) the intensity of band around 1606 cm^{-1} is high for both electron withdrawing and electron donating substituents. In the present case the intensity is high with electron donor groups and low with electron acceptor groups. The intensity of these bands around 1585 cm^{-1} shows the similar vibrational with substitution. The band is slightly stronger than the band near 1605 cm^{-1} . Electron donating substituents increase the intensity of band near 1470 cm^{-1} . The band near 1430 cm^{-1} is unaffected by the nature of the substituents. This trend in the change of intensities has been explained due to the charge disturbance in the molecule (Ahmad et al 1990, Bernhard 1995, Chand^b et al 2021 and Govindarajan et al 2014)

The ring deformation mode involving both stretching and bending of CC band is analogous to e_{1u} (1485 cm^{-1})

mode of benzene. It is divided into two modes under reduced symmetry. They can be detected in the region $1450\text{-}1520\text{ cm}^{-1}$ and $1370\text{-}1438\text{ cm}^{-1}$ respectively and found to be sensitive in small extent (Bellamy 1975, Bernhard 1995, Chand^b et al 2021, Colthup et al 1964 and Varsanyi 1969). The first mode occurs in the infrared spectra of title molecule at 1471 cm^{-1} and at 1474 cm^{-1} in the laser Raman spectra. The second mode is found at 1418 cm^{-1} in infrared spectra and at 1422 cm^{-1} in the laser Raman Spectra for the title molecule. This pair of bands have been identified at 1492 and 1450 cm^{-1} in infrared spectra and at 1491 cm^{-1} in the laser Raman spectra of benzonitrile by Green et al (1971). Some workers (Wilmshurst et al 1957 and Bersani et al 2010) identified this pair of bands at 1482 and 1438 cm^{-1} and one corresponding to mode of benzene at 1310 cm^{-1} in pyridine.

The bands mentioned above for the title molecule are assigned to the coupled CC and CN stretching vibrations. This is supported by literature value (Bersani et al 2010, Colthup et al 1964, Green et al 1971, Rao 1963 and Wilmshurst et al 1957)

These bands arise from similar fundamentals to those which are responsible for the ring breathing modes of benzene. Therefore, it is expected that they will show considerable intensity variations which are due to electronic effect of



the substituents. In benzene the intensity changes can be predicted from a consideration of the magnitude of the change in dipole moment which will be produced by a given group.

In benzene, the band regarding b_{2u} (1310 cm^{-1} mode occurs in the region ($1260\text{-}1290\text{ cm}^{-1}$) In title molecule this mode is identified at 1210/1241 for infrared/laser Raman spectra respectively and assigned to CC stretching. These are in well accordance with the assignments of some workers (Colthup et al 1964, Goel et al 1985, Hussein et al 1977, Kumar^a et al 2022, Mettler 2018 and Rao 1963).

RING BREATHING VIBRATIONS:

Carbon stretching i.e. the ring breathing mode and carbon planar bending vibrations arise from a_{1g} (995 cm^{-1}) and b_{1u} (1010 cm^{-1}) modes of benzene. Ingold (1953) have shown that these modes contain energy very close to each other and both belongs to same symmetry. So, the energies of these modes are modified due to the interaction between them. The ring stretching vibration reduces appreciably depending upon the mass, nature and number of substituent though the bending vibration remains close to 1010 cm^{-1} (Ahmad et al 1990, Bersani et al 2010 and Wilmshurst 1957). On the other hand, the ring breathing vibration is totally symmetric and seems to be polarized and intense in the Raman spectra.

Innes et al (1969) shown the ring breathing vibration at 992 cm^{-1} for pyridine. Hussein (1977) and Bersani et al (2010) have shown this mode at 994 cm^{-1} for 2-chloropyridine whereas Green et al (1977) have shown the same mode at 1038 cm^{-1} in benzonitrile. Thus, in the title molecule the bend each at 1025 cm^{-1} in infrared and laser Raman spectra have been assigned to ring breathing mode. This is supported by literature value (Bersani et al 2010, Bellamy 1975, Hussein et al 1977, Rao 1963 and Varsanyi 1977).

CC-IN-PLANE AND OUT-OF-PLANE BENDING VIBRATION:

The CC in plane bending vibration is obtained from degenerate e_{2g} (608 cm^{-1}) mode of benzene. This mode appears separately under the reduced symmetry and splits into two components. Varsanyi (1977) shown in substituted benzenes that both the components are quite sensitive to mass nature and the number of substituents Green et al (1971) assigned this mode at 547 cm^{-1} and at 461 cm in infrared spectra and at 549 cm^{-1} and 462 cm^{-1} in the laser Raman spectra for benzonitrile. So, the bands of 544 cm^{-1} infrared spectra and at 554 cm^{-1} and 472 cm^{-1} in the laser Raman spectra the title molecule have been assigned to this mode. This is in well accordance with the work of other workers [17,37,48,63,64].



The CC out of plane bending vibrations are derived from nondegenerate b_{2g} (703 cm^{-1}) and degenerate e_{2u} (404 cm^{-1}) modes of benzene. The nondegenerate (703 cm^{-1}) mode has been assigned at $630/631\text{ cm}^{-1}$ in infrared and laser Raman spectra of 4-cyano pyridine. This is supported well with the literature value (Ahmad et al 1990, Green et al 1971, Medhi et al 1990 and Rao et al 1963).

The degenerate e_{2u} (404 cm^{-1}) mode under C_{2v} symmetry have been observed at $403/400\text{ cm}^{-1}$ in infrared and laser Raman spectra of 4-cyano pyridine. It also finds support by the literature value (Bersani et al 2010, Green et al 1971, Rao 1963 and Varsanyi 1969).

CN-GROUP-VIBRATIONS:

Studies on nitriles (Bersani et al 2010, Rao 1963 and Varsanyi 1969) shown that the infrared absorptions appear in the triple bond region $2300\text{-}2200\text{ cm}^{-1}$ and the same was confirmed by Kitson and Griffiths (1952). For mono and dinitriles compounds, the CN frequency also lies between $2260\text{-}2240\text{ cm}^{-1}$. Investigations shows that for the aromatic compound in which CN group was directly attached to the ring absorbed in the region $2240\text{-}2221\text{ cm}^{-1}$. The nature of the other ring substituents affects the frequency to some extent. But the range given includes the absorption shown by the compounds with either electron repelling or electron attracting

substituents. These results are supported well by the work of some workers (Bernhard 1995, Bersani et al 2010, Garoz et al 2019 and Innes et al 1969).

The CN group can be identified in the infrared region provided the intensity is sufficient. It is possible to differentiate between saturated and conjugated nitriles but there is an insufficient difference between alkenyl and aryl nitriles to enable any distinction to be made from the CN frequency.

Large intensity variation is shown by aromatic nitriles in the infrared spectra but in the laser Raman spectra there is no such behavior and the bands are always strong (Bersani et al 2010, Garoz et al 2019, Innes et al 1969 and Rao 1963). In the alkyl series some intensity variations do occur but these are small so the band cannot be recognized easily. In the aromatic nitriles, the bands in the laser Raman spectra are even more clearly marked.

In the present study the CN stretching in-plane and out-of-plane bending vibrations for 4-cyano pyridine in infrared and laser Raman spectra are discussed and are given in Table 1 and their correlation with similar molecules in Table 2.

Bellamy (1975) Shown that CN stretching for aromatic compounds appear in the region ($2240\text{-}2221\text{ cm}^{-1}$). Medhi et al (1990) assigned the band at 2240 cm^{-1} in the infrared and



at 2237 cm^{-1} in the laser Raman spectra to CN stretching vibration for cyano pyridine. Similarly, Green et al (1971) shown this band at 2229 cm^{-1} in infrared spectra and at 2243 cm^{-1} in the laser Raman spectra of benzo nitrile.

So, the very strong bands occurring at 2226 cm^{-1} in the infrared and at 2231 cm^{-1} in laser Raman spectra for 4-cyano pyridine have been assigned to CN Stretching vibrations. This is supported by the work of some investigators (Bellamy 1975, Bersani et al 2010, Ingold 1953 and Mettler 2018).

Some workers (Jacobson et al 1964 and Bersani et al 2010) noted that a band occurs between 380 and 430 cm^{-1} in the aromatic nitric compounds. Jacobson et al (1964) further shown that it belongs to the in plane bending vibration of the whole nitrile group This band was also observed by Bellamy (1975) in the spectra of some p-substituted benzonitriles derivatives but generally only in those cases where the total mass of the other substituent was higher than that of the nitrile group. So, in the present study the bands belong to in-plane bending mode of the whole nitrile group.

Medhi et al (1990) assigned the band at 368 cm^{-1} in infrared spectra and at 376 cm^{-1} in laser Raman spectra to CN in-plane bending vibrations for 3-cyano pyridine. Thus, the bands at 368 cm^{-1} and at 374 cm^{-1} and in the infrared and laser Raman spectra have been assigned to this mode in this present study. This also finds supports from various workers (Mettler 2018, Navati 1977, Rao 1997 and Varsanyi 1969). Jacobson et al (1964) assigned out of plane CN bending mode at 170 cm^{-1} in the laser Raman spectra for aromatic nitriles. So, the bands at 149 cm^{-1} the laser Raman spectra of 4-cyano pyridine have been assigned to CN out-of-plane bending vibrations supported by various workers (Bersani et al 2010, Kumar^a & ^b et al 2022, Mettler 2018, Navati 1977, Rao 1997 and Varsanyi 1969).

TABLE 1
Assignments of Vibrational Frequencies of 4 Cyano Pyridine

Assignments	2-Cyanopyridine		4-Cyanopyridine	
	IR	Raman	IR	Raman



—	3439 m	—	3440 mb	—
ν CH	—	3099 w	—	3090 w
ν CH	3062 S	3067 ms	3068 s	3065 ms
ν CH	3009 vw	—	3005 vw	—
—	2361 ms	—	2365 ms	—
ν CN	2241 vs	2237 vs	2226 vs	2231 vs
—	1975 vvw	—	1970 vvw	—
—	1629 vw	—	1605 w	—
ν CC	1585 vvs	1586 vs	1585 vs	1583 s
ν CC	1529 vvw	—	1563 vs	—
ν CN	1463 vs	—	1471 vs	1474 vvs
ν CC, CH	1438 vs	1438 vvw	1418 vs	1422 vs
β CH	1292 ms	1295 vvw	1246 vvs	1290 vvw
ν (C—C)	1250 ms	1255 w	1210 ms	1241 vvw
β CH	1156 ms	1155 ms	1185 ms	1190 ms
β CH	1093 ms	1062 mw	1082 ms	1046 vvw
β CH	1045 ms	1045 m	1044 ms	1044 ms
ν ring breathing	995 vs	994 vs	1025 s	1028 ms
γ CH	910 w	—	908 w	—
γ CH	786 vvs	784 ms	910 vs	780 m
γ CC	632 m	634 vw	639 vs	631 w
β CC	554 vvs	552 vw	544 vs	554 w
β CC	470 m	—	471 s	472 m
γ CC	402 vvs	493 vvw	403 s	400 vvw
β CN	—	362 w	—	358 w
γ CN	—	176 ms	—	176 s



Lattice vibration	—	161 ms	—	160 ms
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Where ν = Stretching,

β = in-plane-bending,

γ = out-of-plane-bending

vvs = very very strong,

s = strong,

m = medium,

vvw = very very weak,

w = weak,

vs = very strong,

ms = medium strong,

mb = medium broad,

vw = very weak

sh = shoulder

TABLE 2
CN Group Frequencies [infrared and laser Raman] of 4 Cyano
Pyridine and their Correlation with Similar Molecules

Molecules	ν CN		β CN		γ CN	
	IR	Raman	IR	Raman	IR	Raman
2 CP	2238 vs	2237 vs	—	362 w	—	176 ms
3 CP	2229 vs	2238 vs	—	358 w	—	176 ms
4 CP	2226 vs	2231 vs	368 mw	374 w	149 mvv	149 s
B N	2229 vs	2243 vs	379 m	379 w	178 s	172 vs
P—FBN	2237 s	2235 vs	4025 s	—	158 m	162 s
P—CBN	2236 s	—	—	302 m	192 m	157 m
P—BBN	2237 s	2229 vs	274 w	277 m	140 m	161 s
P—MBN	2230 s	2228	344 m	345	156 s	141 ms



2,4—CFBN	2233 vs	2235 vs	550 ms	545 ms	—	145 ms
3,4—FBN	2233 s	2240 vs	592 s	600 ms	—	145 m
2,5—FMBN	2252 s	2250 vs	579 ms	—	—	145 m
5,2—FMBN	2224 s	2220 vs	591 s	585 ms	—	130 m
3—ABN	2240 ms	—	560 m	—	220 s	—

Where 4-CP = 4 Cyano pyridine (title molecule), BN = Benzonitrile,

P-FBN = Para Fluoro benzonitrile, P-CBN = Para chloro benzonitrile,

P-BBN = Paral Bromo benzonitrile, P-MBN = Para Methyle benzonitrile,

2,4-CFBN=2-Chloro-4-fluoro benzonitrile, 3,4-CFBN=3-Chloro-4-fluoro benzonitrile

2,5-MBN = 2 fluoro-5 methyl benzonitrile,

5,2-MBN = 5 fluoro-2 methyl benzonitrile

3-ABN =3 Amino methyl benzonitrile

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

s = strong, vs = very strong, m = medium,

ms = medium strong, w = weak, mw = medium weak,



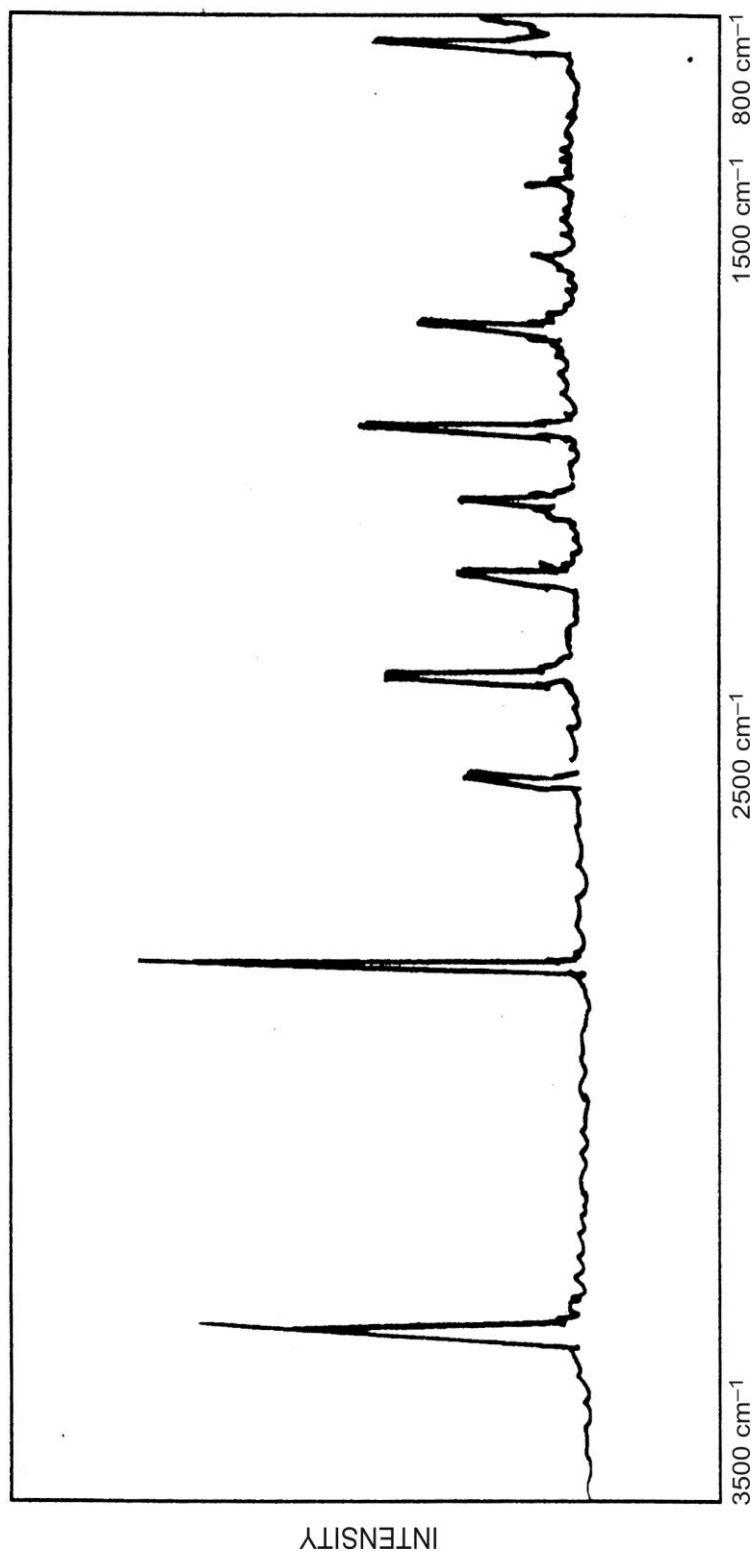


Figure 2: Infrared Spectrum of 4 Cyano Pyridine

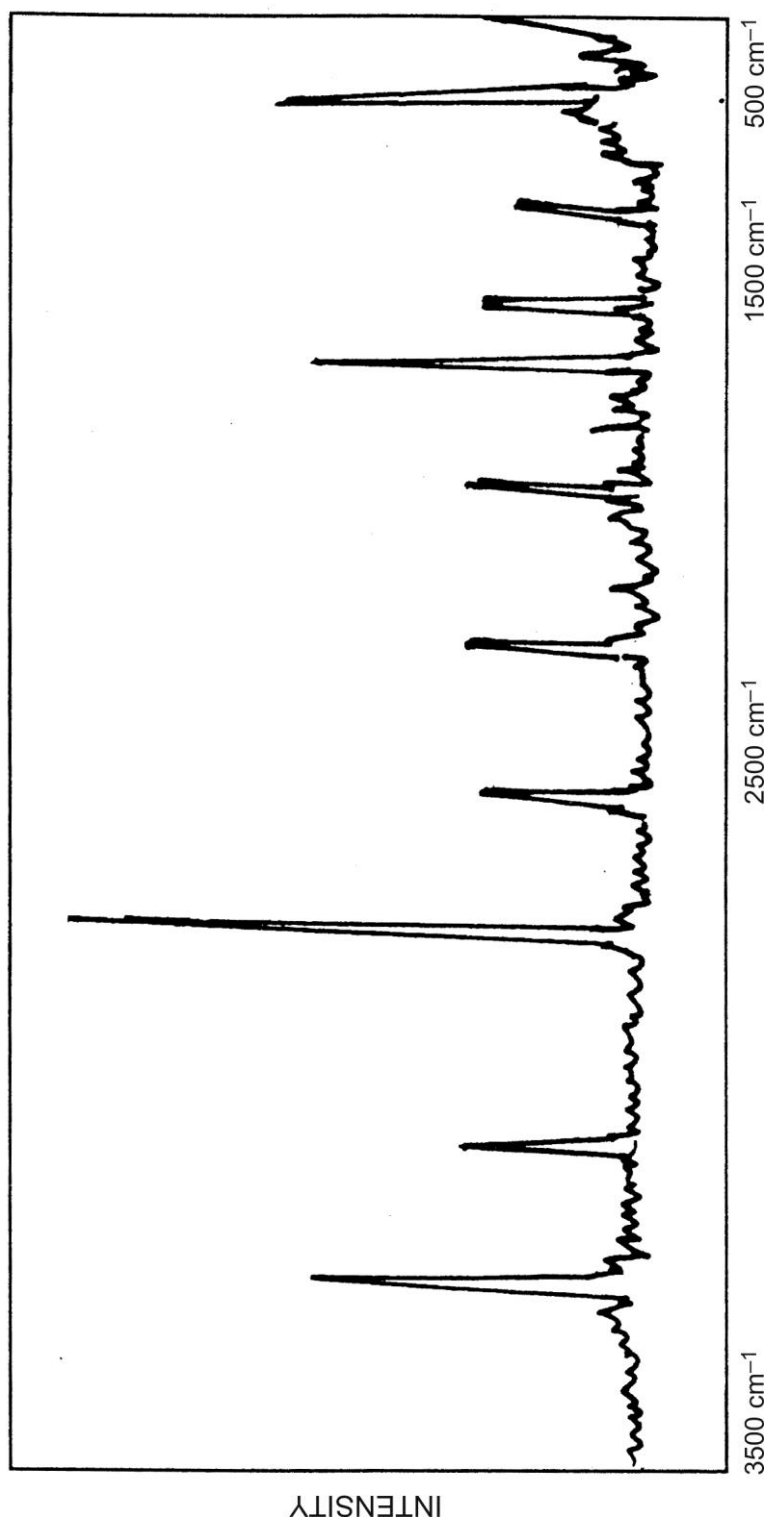


Figure 3: Laser Raman Spectrum of 4 Cyano Pyridine

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