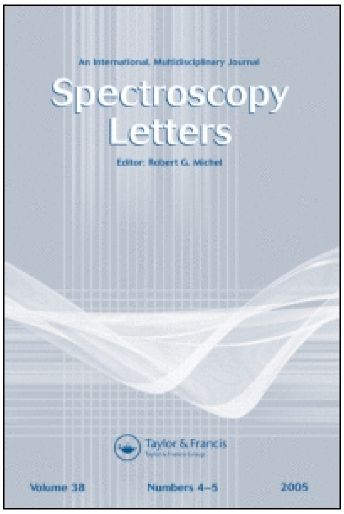

Spectroscopy Letters
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597299

Vibrational Spectra of α-Pyrazinamide and ^{15}N-α-Pyrazinamide

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To cite this Article Delgado, M. J. Martín , Márquez, F. , Suero, M. I. and Marcos, J. I.(1988) 'Vibrational Spectra of α-Pyrazinamide and ^{15}N-α-Pyrazinamide', Spectroscopy Letters, 21: 8, 841 — 852
To link to this Article: DOI: 10.1080/00387018808082346
URL: http://dx.doi.org/10.1080/00387018808082346

SPECTROSCOPY LETTERS, 21(8), 841-852 (1988)

VIBRATIONAL SPECTRA OF α-PYRAZINAMIDE AND ^{15}N-α-PYRAZINAMIDE

KEY WORDS: Infrared, Raman, Isotopic efects, Pyrazinamide

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ABSTRACT

α-Pyrazinamide and its α-Pyrazinamide-d_2 as well as the ^{15}N-isotopic derivative were synthesized with an isotopic content of 99.4% and their Raman and infrared spectra were recorded and assigned on the basis of isotopic shifts.

INTRODUCTION

Although pyrazinamide (pyrazín-2-carboxamide) and its derivatives are of biological interest[1-3] their vibrational spectra have not been thoroughly investigated. Partial assignments of the infra-

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red spectrum of pyrazinamide and pyrazinamide-d_2 have been reported[4] but being limited to some amide group vibrations, on the other hand the lack of infrared data below 800 cm^{-1} has precluded.complete assignment. No study of the Raman spectra of pyrazinamide and pyrazinamide-d_2 as well as of the ^{15}N isotopic derivative have been published uo to now. Prior to this work, a previous study of the vibrational spectra of $^1H_4$-pyrazine and $^2H_4$-pyrazine[5-6] as well as the methylpyrazines[7] and pyrazinoic acid and his ion[8] that have provided a guide for the assignations of ring vibrations. On the other hand, the crystal structure of pyrazinamide has been examined by X-ray analysis and is known to appear in four different crystalline modifications, namely α-, β-, γ- and δ-pyrazinamide[9]. The existence of several modifications of carboxamides will probably be due to the difference of the possible linking configurations of hydrogen bond systems. The α-form (α-PCA) is monoclinic and space group $P2_{1/a}$ (C^5_{2h}) with four molecules in the unit cell. The pyrazine ring is completely planar and makes an angle about 6º to the amide group[10-11]. The molecules are conected by N-H-O hydrogen bonds forming dimers across the centre of symmetry, and there are indications of N-H-N hydrogen bonds linking the dimers into endless chains.

In view of the biological significance of pyrazinamide, and the interesting possibilities for hydrogen bond structures in this compound, the investigation of the vibrational spectra was undertaken. This paper presents the Raman and infrared spectra of natural α-PCA and the infrared spectrum of α-PCA-d_2 as well as the infrared spectrum of ^{15}N isotopic derivative with an isotopic content of 99.4%. This paper also presents tentative vibrational assignments on the basis of group frequency considerations and isotopic frequency shifts produced by ^{15}N substitution and ^2H substitution.

EXPERIMENTAL

The isotopic compound ^{15}N-α-PCA has been synthesized with $^{15}NH_4Cl$ with an isotopic content of 99.4%. First methylpyrazinecarboxilate was synthesized according to the classical method of Hall and Spoerri[12] including some modifications to operate in semimicro scale. The purity of both normal and isotopic compound was satisfactorily verified by contrasting their infrared spectrum against a standard one. Deuterated pyrazinamide was obtained by adding an excess of D_2O (99.4%) and double crystallization from the same solvent in vacuum over P_2O_5. Infrared analysis showed that NH_3 group is deuterated more than 97%. Infrared spectra were recorded on potassium bromide and polyethylene discs on a Beckman 4260 spectrophotometer in the 4000-200 cm^{-1} region. Standards for wavenumber determination were polystyrene film and indene+camphor+cyclohexanone mixtures as described in ref.[13]. The experimental error was ± 0.5 cm^{-1}. Raman spectra were recorded with a Jobin Yvon Ramanor U-1000 spectrometer by using the 5145 A exciting line from Ar^+ Spectra Physics (model 2020/3). Calibrations were made by using either plasma lines from the laser or from an Ne lamp. According to the experimental conditions of recording and measuring the frequencies have an estimated error of ± 2 cm^{-1} in the Raman frequencies.

The experimental results are summarized in Tables 1, 2 and 3 where frequencies, isotopic shifts and assignments can be seen.

RESULTS AND DISCUSSION

The assignments were based on the approach in which the vibrational spectra of pyrazinamide are assumed to be the superposition of bands corresponding to the $-CONH_2$ group and pyrazine. On this basis, the ring vibrations have been classified according to symmetry of individual molecules, that is to say C_s, and the substituents vibrations, provided that the $-CONH_2$ groups are hydrogen-bonded to form centrosymmetric dimers of symmetry C_{2h}, we have considered that this point group is the relevant one to classify normal vibrations involving the $-CONH_2$ groups into symmetry species. Therefore, each characteristic mode of the carboxamide groups will be either symmetric or antisymmetric with respect to the centre of symmetry. According to this the characteristic vibrations can be classified as follows:

-Symmetry species A_g and B_u: One of each of $\nu(C=O)$, $\nu(CN)$, $\nu_s(NH_2)$, $\nu_{as}(NH_2)$, $\delta(OCN)$, $r(OCN)$, $\delta(NH_2)$ and $r(NH_2)$ in each species.

TABLE 1

Summary of the Frequencies, Isotopic Shifts and Proposed Assignments for the Fundamentals Bands of Vibrational Spectrum of Pyrazinamide in the 4000-1000 cm^{-1} Region.

i.r. ^{14}N		i.r. ^{15}N			i.r. $^{14}ND_2$		Raman ^{14}N		
ν	I	ν	I	$\Delta\nu$	ν	I	ν	I	Assignment
							3430.7	w	$\nu_{as}(NH_2),A_g$
3415.0	vs	3407.5	vs	7.5					$\nu_{as}(NH_2),B_u$
3163.0	s	3156.0	s	7.0					$\nu_s(NH_2),B_u$
							3160.0	vw	$\nu_s(NH_2),A_g$
3091.5	w	3090.4	w	1.1	3093.2	vw	3090.3	w	$\nu(CH),A'$
3067.0	w	3066.8	w	0.2	3069.6	w	3066.8	m	$\nu(CH),A'$
3053.3	w	3053.0	w	0.3	3053.9	w	3053.2	m	$\nu(CH),A'$
					2554.6	s			$\nu_{as}(ND_2),B_u$
					2375.6	s			$\nu_s(ND_2),B_u$
1712.4	vs	1708.0	vs	4.4	1701.0	vs			Amide I,B_u
							1671.5	m	Amide I,A_g
1612.7	s	1608.6	s	4.1					Amide II,B_u
							1606.6	sh	Amide II,A_g
1582.9	m	1583.6	m	0.7	1582.4	m	1582.0	vs	8a;ν_{ring},A'
1523.4	m	1523.5	m	0.1	1523.7	m	1524.3	s	8b;ν_{ring},A'
1479.7	w	1479.4	w	0.3	1480.1	w	1487.0	m	19a;ν_{ring},A'
							1396.5	sh	19b;ν_{ring},A'
							1381.1	w	Amide III,A_g
1379.0	vs	1376.4	vs	2.6	1379.9	vs			Amide III,B_u
							1296.4	w	$\nu(CX),A'$
					1229.8	w			Amide II,B_u
1182.9	m	1180.3	m	2.6	1181.5	w	1181.7	w	$\delta(CH),A'$
1165.8	m	1166.2	m	0.4	1165.7	m	1166.8	w	14;ν_{ring},A'
1087.6	m	1080.8	m	6.8					$r(NH_2),B_u$
							1080.8	m	$r(NH_2),A_g$
1053.9	s	1053.5	s	0.4	1054.0	s	1052.1	vs	$\delta(CH),A'$
1023.9	s	1023.8	s	0.1	1025.0	s	1026.0	vs	12;δ_{ring},A'

TABLE 2

Summary of the Frequencies, Isotopic Shifts and Proposed Assignments for the Fundamentals Bands of Vibrational Spectrum of Pyrazinamide Below 1000 cm^{-1}.

i.r. ^{14}N		i.r. ^{15}N			i.r. ^{14}ND$_2$		Raman ^{14}N		
ν	I	ν	I	Δν	ν	I	ν	I	Assignment
							956.1	vw	γ(CH),A"
					919.4	m			r(ND_2),B_u
870.3	s	870.1	s	0.2	868.0	s	867.5	m	γ(CH),A"
807.9	sh	807.5	sh	0.4	809.0	w	806.4	s	1;ν_{ring},A'
785.5	s	785.0	s	0.5	775.0	s	777.8	w	4;γ_{ring},A"
762.8	vw	761.6	vw	1.2					t(NH_2),A_u
					716.8	w			t(ND_2),A_u
700.5	vw	700.0	vw	0.5	700.0	vw			δ(OCN),B_u
669.7	s	667.2	s	2.5					ω(NH_2),A_u
							660.6	w	ω(NH_2),B_g
618.1	sh	618.1	sh	0.0			617.0	w	6a or 6b,A'
					600.0	w			ω(ND_2),A_u
543.6	sb	541.8	sb	1.8	540.0	sb			r(OCN),B_u
520.0	sh	517.5	sh	2.5					γ(OCN),B_u
434.0	s	433.4	s	0.6	430.0	s	416.0	w	16b;γ_{ring},A"
380.1	w	379.7	w	0.4	375.3	w	380.4	w	δ(CX),A'
							173.6	s	γ(CX),A"
							116.3	vs	t(C-$CONH_2$),A"

-Symmetry species A_u and B_g: One of each γ(OCN), ω(NH_2), t(NH_2) and torsional mode.

Concerning to ring vibrations they can be as follows:

-Symmetry species A': 1,6a,6b,8a,8b,12,14,19a,19b, three ν(CH), three δ(CH), one ν(CX) and one δ(CX).

-Symmetry species A": 4,16a,16b, three γ(CH) and γ(CX).

TABLE 3

Summary of the Frequencies,Isotopic Shifts and Proposed Assignments for the Combinations and Differences Bands of Vibrational Spectrum of Pyrazinamide.

i.r. ^{14}N		i.r. ^{15}N			i.r. $^{14}ND_2$		
ν	I	ν	I	$\Delta\nu$	ν	I	Assignment
3290.0	m	3281.7	m	8.3	3294.0	m	8a+Amide I
3205.0	sh	3198.3	sh	6.7			8a+Amide II
2927.0	w	2927.0	w	0.0			8b+19b,A'
					2926.0	m	$\nu_{as}(ND_2)+\delta(CX)$
2855.5	vw	2854.3	vw	1.2	2853.0	vw	19a+Amide III
2746.5	vw	2739.3	vw	7.2			$\nu_{as}(NH_2)-\omega(NH_2)$
					2744.8	vw	8b+Amide II
					2455.8	sh	$\nu(CH)-\omega(ND_2)$
1974.0	vw	1974.0	vw	0.0	1973.0	vw	14+1,A'
1943.7	vw	1940.5	vw	3.2			$\delta(CH)+t(NH_2)$
1911.4	vw	1911.0	vw	0.4	1911.3	vw	$8b+\delta(CX)$,A'
1854.4	vw	1854.0	vw	0.4			$19a+\delta(CX)$,A'
1826.5	vw	1826.0	vw	0.5			$\gamma(CH)+\gamma(CH)$,A'
1466.4	sh	1466.1	sh	0.3	1467.6	sh	$\nu(CH)-8a$,A'
986.6	vw						$\gamma(CH)+t(CC)$,A'

Wilson's[14] notation has been used for the assignments of ring vibrations which are associated with the benzene frame.

ASSIGNMENTS OF THE VIBRATIONAL SPECTRUM.

In order to carry out an assignment of the vibrational spectrum, we classified the normal vibrations as: a) Vibrations of the pyrazine ring, b) ring-substituent vibrations and c) vibrations of the substituent. The assignments proposed are based on experimental data including the isotopic shifts of ^{15}N and ^{2}H as well as on the correlation of the pyrazinamide spectrum with that of pyrazine, methylpyrazine and pyrazinoic acid studied by us.

a) Vibrations of the pyrazine ring.-

With respect to the in-plane vibrations, we have assigned the three ν(CH)A' modes to the weak bands recorded on the low frequency side of stretching NH_2 band in the i.r. spectrum at 3091.5, 3067 and 3053.3 cm^{-1} which are not sensitive to the isotopic substitution. In the Raman spectrum they have been recorded at 3090.3, 3066.8 and 3053.2 cm^{-1} respectively. Both the 8ab and 19ab pairs are recorded more or less at the same frequency as in the pyrazine spectrum, though the 19b mode is hidden in the Amide III band of i.r. spectrum, recording at 1396.5 cm^{-1} of Raman spectrum. The same occurs for mode 12 which generally appears at a very steady frequency and is the strongest Raman band in this region of the spectrum, it is recorded at 1023.9 and 1026 cm^{-1} in the i.r. and Raman spectra respectively. On the other hand, mode 1, recorded at 1016 cm^{-1} in the pyrazine spectrum, now appears at 806.4 cm^{-1} due to substitution effects. With regard to mode 14 is assigned by correlations with pyrazinoic acid to a band recorded at 1165.8 and 1166.8 cm^{-1} in the i.r. and Raman spectra. Concerning to assignments of the pair 6ab, it is less certain because in this zone of the spectrum are expected characteristic vibrations of the substituent group, both have been assigned to the bands at 618.1 and 617 cm^{-1} of i.r. and Raman spectra respectively, in the basis that they are the only bands which are not sensitive to the isotopic ^{15}N substitution.

Finally, only two δ(CH) modes have been assigned to the bands recorded at 1182.9 and 1053.9 cm^{-1} of i.r. spectra with the Raman partners appearing at 1181.7 and 1052.1 cm^{-1} respectively though the assignment of the higher frequency is less certain because it presents a isotopic shift higher for a C-H in-plane deformation, because of this, this can be, very probably, a combination involving the nitrogen atom of the substituent.

With respect to the out-of-plane vibrations which should be of A" symmetry, we have assigned two γ(CH) modes to the bands recorded at 956.1 and 867.5 cm^{-1} in the Raman spectrum, the latter is assigned to the strong band recorded at 870.3 cm^{-1} in the i.r. spectrum, the first γ(CH) mode is seen only in the Raman spectrum. Concerning to mode 4, has been assigned to the strong band at 785.5 cm^{-1} in the i.r. spectrum and 777.8 cm^{-1} of Raman spectrum.

Finally, the 16ab pair has been observed by us only in the band at 434 and 416 cm^{-1} in the i.r. and Raman spectra respectively, which we have assigned to mode 16b since this mode is characterized by a strong band in the i.r. spectrum.

b) Ring-substituent vibrations.-

For vibrations which involve the ring substituent bond, that is to say, ν(CX)A', δ(CX)A' and γ(CX)A" modes, we have assigned the stretching mode according to the interval of frequency to a weak Raman band at 1296.4 cm^{-1}, but it does not appear in the infrared spectrum. Concerning to bending modes which are expected in the low frequency region, a careful examination of the spectra recorded in polyethylene matrix reveals the presence of a weak band at 380 cm^{-1} in the i.r. spectrum, which we have assigned tentatively to vibration corresponding to the in-plane bending mode. The corresponding Raman line appears to the same frequency.

Finally, the C-X out-of-plane bending mode is expected in the lowest frequency zone. The strong Raman band at 173.6 cm^{-1} is identified with this mode. The i.r. partner could not be recorded in our case because it is out of the spectral range of our instrument.

c) Vibrations of the substituent.-

Comparison of the i.r. and Raman spectra of this compound show that they are clearly noncoincident. The hydrogen bonding in α-PCA is extensive and no doubt the molecule exist as a hydrogen-bonded chain of some complexity.

-Stretching vibrations.- Assuming the point group C_{2h} as relevant for any $CONH_2$ characteristic vibration, two different asymmetric and symmetric N-H stretching modes must be considered. The $\nu_{as}(NH_2)$ of B_u symmetry must be assigned to the strong i.r. band at 3415 cm^{-1} with an isotopic shift of 7.5 cm^{-1} and the A_g one to the weak Raman band at 3430.7 cm^{-1}. Likewise the vibrations $\nu_s(NH_2)$ B_u and

A_g, appear in the i.r. and Raman spectra but at different frequencies as can be seen in Table 1. Isotopic shifts of ^{15}N substitution is greater in the $\nu_{as}(NH_2)$ band than in the $\nu_s(NH_2)$, as it is generally observed in primary amides[15]. On the other hand, the corresponding values of the ratio $\nu_{as}NH_2/\nu_{as}ND_2$ and ν_sNH_2/ν_sND_2 were 1.33 in both modes in good agreement with[4]. At lower frequencies it has been identified the primary Amide I band -in which the $\nu(C{=}O)$ vibration predominates[16]- the B_u mode is assigned to a very strong band at 1712.4 cm^{-1} of i.r. spectrum with an isotopic shift of 4.4 cm^{-1}. The magnitude of the isotopic shift indicates an important participation of a vibration moving the nitrogen nucleus, which in agreement with[17] must be $\delta(NH_2)$ and $\nu(CN)$. Likewise the A_g mode is assigned to a band at 1671.5 cm^{-1} of the Raman spectrum. The comparison of the i.r. and Raman spectra of this vibrations show them to be clearly noncoincident. The data are consistent with hydrogen-bonded chains, their carboxamide dimeric units having a local center of symmetry. On the other hand, the Amide III band -in which $\nu(CN)$ predominates- is assigned to the 1379 cm^{-1} band of i.r. spectrum in agreement with[4], with an isotopic shift of 2.6 cm^{-1}. The mode active in Raman is assigned to a weak band at 1381.1 cm^{-1}.

-In plane bending vibrations.- Among the in-plane bending vibrations, at a higher frequency appears the primary Amide II band -in which $\delta(NH_2)$ predominates-. According to the observed isotopic shifts and the corresponding values of the ratio $\delta(NH_2)/\delta(ND_2)$ has been assigned to a strong band at 1612.7 cm^{-1} in the i.r. spectrum. The corresponding deuterated amide group appears at 1229.8 cm^{-1} in good agreement with[4]. The Raman active mode, A_g symmetry is assigned to a shoulder at 1606.6 cm^{-1}. The magnitude of the isotopic shift in the deuterated compound shows a greater participation of $\delta(NH_2)$ mode in the moving of vibration. On the other hand, near 1500 cm^{-1} in the i.r. spectrum appears a band resulting from deuteration, this absorption band was considered to be a deformation band[18] for ND, caused by a half-deuterated amino group, this band was also observed for benzamide[4]. Concerning to $r(NH_2)$ vibrations, we have found some controversy regarding the assignments reported by Yoshida[4] who has observed two frequencies at 1182 and 1088 cm^{-1} for $r(NH_2)$ vibrations in the i.r. spectrum, and which when it was deuterated, only one band was observed. However, we have given a different interpretation to this, we think that this firt band is the (CH)A' mode which has been observed by us at 1182.9 cm^{-1} is in good agreement with[7-8]. Therefore the latter can be assigned to $r(NH_2)$ which has been recorded by us at 1087.6 cm^{-1} in the i.r. spectrum and at 919.4 cm^{-1}, with a displacement ratio of 1.18 in the deuterated compound. On the other hand, the isotopic shift ^{15}N of 6.8 cm^{-1} is in good agreement with the previous assignments which assume the NH_2 rocking mode predominating in this band[17]. The corresponding Raman band of A_g symmetry is recorded at 1080.8 cm^{-1}. The assignments seem to us to be more realistic that these of Yoshida.

Finally, only two r(OCN) and δ(OCN) vibrations remain to be assigned. The rocking vibration generally appears with a strong intensity in the i.r. spectrum, we have assigned it to the broad band at 543.6 cm^{-1} with a isotopic shift of 1.8 cm^{-1} in agreement with other amides[19,20]. The Raman active mode has not been observed. Concerning the δ(OCN) vibration, some authors[21,22] assume that this mode appears together γ(OCN) mode, while other authors assign them separatedly[23]. Both vibration modes have been observed by us separatedly according to the interval of frequencies[24]. In the range of apparition of δ(OCN) mode there are recorded in the i.r. spectrum two weak bands at 762.8 and 700.5 cm^{-1}, the first band is absent in the deuterated compound, thereby it can be assigned to $t(NH_2)$ mode, therefore, the δ(OCN) vibration must be assigned to the 700.5 cm^{-1} band, though this assignation is less certain because it is a very weak band.

-Out-of-plane vibrations.- Corresponding to this group are expected the $t(NH_2)$, $\omega(NH_2)$, γ(OCN) and t(C-C') modes. The first mode is barely sensitive to the isotopic shift since the nitrogen atom practically does not move at all, while in the $\omega(NH_2)$ mode it displaces out-of-plane, so that, it will shift towards a lower frequency in the ^{14}N-^{15}N substitution. On the other hand, both modes must be sen sitives by the deuteration. On this basis, and according to the interval of frequencies for this vibrations, we have assigned the $t(NH_2)$ mode to a weak band at 762.8 cm^{-1} in the i.r. spectrum with an isotopic shift of 1.2 cm^{-1}. We have not found any Raman band which could be assigned to $t(NH_2)B_g$. The $\omega(NH_2)A_u$ vibration which must be sensitive to the ^{15}N substitution has been assigned to a strong band at 669.7 cm^{-1} in the i.r. spectrum with an isotopic shift of 2.5 cm^{-1} and $\omega(NH_2)B_g$ mode at 660.6 cm^{-1} in the Raman spectrum. The corresponding $t(ND_2)$ and $\omega(ND_2)$ modes both appearing in the i.r. spectra at 716.8 and 600 cm^{-1} with a displacement ratio of 1.06 and 1.12 respectively. Concerning the $\gamma(OCN)$ mode, we have assigned it to a shoulder recorded at 520 cm^{-1}, together to a broad band assigned to the rocking mode, with a isotopic shift of 2.5 cm^{-1}. The Raman active mode has not been observed.

Finally, the vibration of torsion $t(C\text{-}CONH_2)$ which is expected to appear at a very low frequency can be assigned to the strong band at the lowest frequency in the Raman spectrum, 116.3 cm^{-1} in this case.

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Date Received: 06/16/88
Date Accepted: 07/22/88